

## MARKOV JUMP PROCESSES IN MODELING COALESCENT WITH RECOMBINATION

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Genetic recombination is one of the most important mechanisms that can generate and maintain diversity, and recombination information plays an important role in population genetic studies. However, the phenomenon of recombination is extremely complex, and hence simulation methods are indispensable in the statistical inference of recombination. So far there are mainly two classes of simulation models practically in wide use: back-in-time models and spatially moving models. However, the statistical properties shared by the two classes of simulation models have not yet been theoretically studied. Based on our joint research with CAS-MPG Partner Institute for Computational Biology and with Beijing Jiaotong University, in this paper we provide for the first time a rigorous argument that the statistical properties of the two classes of simulation models are identical. That is, they share the same probability distribution on the space of ancestral recombination graphs (ARGs). As a consequence, our study provides a unified interpretation for the algorithms of simulating coalescent with recombination, and will facilitate the study of statistical inference on recombination.

**1. Introduction.** Genetic recombination is an important mechanism which generates and maintains diversity. It is one of the main sources providing new genetic materials that allow nature selection to carry on. In various

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Received January 2014; revised April 2014.

<sup>1</sup>Supported by the National Center for Mathematics and Interdisciplinary Sciences (NCMIS).

<sup>2</sup>Supported by 973 project (2011CB808000), NSFC Creative Research Groups (11021161) and the Fundamental Research Funds for the Central Universities (2011JBZ019).

*AMS 2000 subject classifications.* Primary 60J25, 65C60; secondary 92B15, 92D25, 60J75.

*Key words and phrases.* Markov jump process, coalescent process, random sequence, conditional distribution, genetic recombination, ancestral recombination graph, back-in-time algorithm, spatial algorithm.

This is an electronic reprint of the original article published by the Institute of Mathematical Statistics in *The Annals of Statistics*, 2014, Vol. 42, No. 4, 1361–1393. This reprint differs from the original in pagination and typographic detail.

population genetic studies, such as DNA sequencing, disease study, population history study, etc., recombination information plays an important role. On the other hand, recombination adds much more complexity and makes statistical inference of some evolutionary parameters more difficult. In the last two decades, some simulation models generating graphs, called ancestral recombination graphs (ARGs), based on coalescent processes have been developed to study recombination. However, none of the existing simulation models is perfect and each has its own advantages and disadvantages.

Historically, a model generating the genealogical relationship between  $k$  sampled sequences from a population with constant size without recombination was first described by Watterson (cf. [17]), and further developed into the theory of the coalescent by Kingman (cf. [12, 13]). A model describing the evolution of infinite-site sequences subject to both coalescence and recombination in a population was first introduced by Hudson (cf. [10]). In his setup, a combined coalescent and recombination process is followed back in time until all nucleotide positions in the extant sequence have one common ancestral nucleotide. The resulting structure is no longer a tree but a graph, which was later named as ARG by Griffiths and Marjoram, who gave in [8] more details on ARG and embedded ARG in a birth–death process with exponentially distributed and independent waiting times for coalescent and recombination events. The ARG described by Griffiths and Marjoram is simple but in many cases unnecessarily time consuming to simulate. Because an “ancestral” sequence in the birth–death process may have no genetic material in common with a sequence descended from it. Adjusting the above shortcoming, Hudson proposed a more efficient algorithm *ms* (cf. [11]) which is now a commonly used computer program to simulate coalescence. Hudson’s program generates ARG back in time from the present. Due to the Markov property of the process, the algorithm is computationally straightforward and simple. But it is not possible to reduce the computation further, and it is hard to approximate the computation. On the other hand, Wiuf and Hein proposed an alternative algorithm that moves along the sequences and modifies the genealogy as recombination breakpoints are encountered (cf. [18]). It begins with a coalescent tree at the left end of the sequence, and adds more different local trees gradually along the sequence, which form part of the ARG. The algorithm terminates at the right end of the sequence when the full ARG is determined. Wiuf and Hein’s algorithm will produce some redundant branches in ARG. Its performance is not so good in comparison with *ms*. But the spatially moving program is easier to approximate. Based on the idea of constructing ARG along sequences, there have been some approximation algorithms, such as SMC, SMC’, and MaCS (cf. [1, 14, 15]). Wiuf and Hein’s spatial approach of simulating genealogies along a sequence has a complex non-Markovian structure in that the distribution of the next genealogy depends not just on the current genealogy,

but also on all previous ones. Therefore, the mathematical formulation of spatial algorithm is cumbersome, and up to date all the comparisons and discussions between spatial algorithms and *ms* (back-in-time algorithm) are based on simulation studies. There is no rigorous argument showing that the ARG generated by a spatial algorithm can share the same probability distribution as the ARG generated by a back-in-time algorithm.

In our recent joint research with scientists in computational biology, we proposed a new model describing coalescent with recombination, and developed a new algorithm based on this new model. Our algorithm is also a spatial algorithm. But we have improved Wiuf and Hein's program in that our algorithm does not produce any redundant branches which are inevitable in Wiuf and Hein's algorithm. In generating ARGs, our algorithm has comparable performance with the algorithm *ms*. In addition, our method can generate ARGs that are consistent with the sample directly. Moreover, we can show that the existing approximation methods (SMC, SMC', MaCS) are all special cases of our algorithm. For details, see our joint paper [16].

In this paper, we further study the statistical properties of our new model. In particular, we prove rigorously that the statistical properties of the ARG generated by our spatially moving model and that generated by a back-in-time model are identical, that is, they share the same probability distribution on the space of ARGs (cf. Theorem 8 below). Since the existing approximations by spatial methods (SMC, SMC', MaCS) are all special cases of our algorithm, consequently our study provides a unified interpretation for the algorithms of simulating coalescent with recombination, and will facilitate the study of statistical inference of recombination.

The remainder of this paper is organized as follows. As a necessary preparation, in Section 2 we investigate in detail the back-in-time model. In Section 2.1, we describe briefly a typical back-in-time model for simulating coalescent processes with recombination. Then we study the state space of the Markov jump process behind the model. In Section 2.2, we construct a Markov jump process corresponding to the typical back-in-time algorithm. In Section 2.3, we show that with probability one, a path of the Markov jump process constitutes an ARG. We then explore some properties of the space  $G$  of ARGs. It is worth pointing out that although Section 2 is a necessary preparation, indeed our investigation is new and the results obtained in this section have interests by their own. In particular, we believe that the probabilistic ARG space  $(G, \mathcal{B}(G), P)$  obtained in Theorem 1 will be very useful elsewhere. In Section 3, we present our main results on the spatially moving model. In Section 3.1, we define and study a random sequence  $\{(S_i, Z^i), i \geq 0\}$  on the probabilistic ARG space  $(G, \mathcal{B}(G), P)$ , which is important for modeling our spatial algorithm. We first define the random sequence  $\{(S_i, Z^i), i \geq 0\}$  and study its measurable structure. We then discuss and derive the distributions of  $S_i$  and  $Z^i$ . The derivations of the suc-

cessive conditional distributions of the involved random variables are very complicated. Some cumbersome derivations are moved to the supplementary article [4]. In Section 3.2, we describe our model of spatially moving algorithm and study its statistical property. We first briefly describe the algorithm *SC* (Sequence Coalescence simulator) of our spatial model. Afterward, we give some explanation of the algorithm. Finally, we reach the main goal of the paper. We show that the statistical property of the ARG generated by our spatially moving model recently proposed in [16] is identical with the one generated by the typical back-in-time model discussed in Section 2, that is, they share the same probability distribution on the ARG space (see Theorem 8). In Section 4, we present the proofs of the main results along with some technical lemmas. To reduce the length of the paper, the proofs of the results in Section 2 as well as part of the results in Section 3 are moved to the supplementary article [4].

## 2. Preparation: Investigation on the back-in-time model.

2.1. *State space of back-in-time model.* We start our discussion by describing the state space of the Markov jump process behind the model of a typical back-in-time algorithm. Following Griffiths and Marjoram (cf. [7, 8]), in our model a gene or a DNA sequence is represented by the unit interval  $[0, 1)$ . The model is derived from a discrete Wright–Fisher model in which, when looking back in time, children in a generation choose one parent with probability  $1 - r$ , or two parents with probability  $r$ ; the latter means that a recombination event occurs. If recombination occurs, a position  $S$  for the breakpoint is chosen (independent from other breakpoints) according to a given distribution, and the child gene is formed with the gene segments  $[0, S)$  from the first parent and  $[S, 1)$  from the second parent. A continuous time model is obtained by first fixing the population size  $2N_e$  and then letting  $N_e \rightarrow \infty$ . Time is measured in units of  $2N_e$  and the recombination rate per gene per generation  $r$  is scaled by holding  $\rho = 4N_e r$  fixed. The limit model is a continuous time Markov process with state space described as below.

Let  $\mathcal{P}_N$  be the collection of all the subsets of  $\{1, 2, \dots, N\}$ . We endow  $\mathcal{P}_N$  with the discrete metric which will be denoted by  $d_p$ . Throughout this paper, we shall fix  $N$  and shall hence simply write  $\mathcal{P}$  for  $\mathcal{P}_N$ . We denote by  $\mathcal{S}_{[0,1)}(\mathcal{P})$  the family of all the  $\mathcal{P}$ -valued right continuous piecewise constant functions on  $[0, 1)$  with at most finitely many discontinuity points. An element  $f \in \mathcal{S}_{[0,1)}(\mathcal{P})$  may be expressed as  $f = \sum_{i=0}^m f(a_i) I_{[a_i, a_{i+1})}$  with  $0 = a_0 < a_1 < \dots < a_m < a_{m+1} = 1$ , which means that  $f$  takes value  $f(a_i) \in \mathcal{P}$  on the semiclosed interval  $[a_i, a_{i+1})$  for each  $i$ .

DEFINITION 1. A finite subset  $x = \{f_1, f_2, \dots, f_k\}$  of  $\mathcal{S}_{[0,1)}(\mathcal{P})$  is said to be a state, and is denoted by  $x \in E$ , if and only if  $\{f_j(s) : f_j(s) \neq \emptyset, j =$

$1, 2, \dots, k$  form a partition of  $\{1, 2, \dots, N\}$  for each  $s \in [0, 1)$ , and  $f_j \not\equiv \emptyset$  for each  $j = 1, 2, \dots, k$ .

The totality  $E$  of all the states will serve as a state space of the Markov process behind our algorithm. The process takes values in  $E$ , starts at the present and traces back in time. At the present time  $X(0) = \varpi$ , here

$$(2.1) \quad \varpi := (h_1, h_2, \dots, h_N) \quad \text{with } h_j = \{j\}I_{[0,1)} \text{ for each } j = 1, 2, \dots, N,$$

representing that the algorithm starts from  $N$  sample lineages of *DNA* sequences. Starting from the present and looking back in time, if  $X(t) = x$  with  $x = (f_1, f_2, \dots, f_k) \in E$ , then it represents that at time point  $t$ , there are  $k$  ancestral lineages (i.e., there are  $k$  lineages which carry the ancestral materials of the samples); if  $f_j \in X(t)$  is expressed as  $f_j = \sum_{i=0}^m f_j(a_i)I_{[a_i, a_{i+1})}$ , then, for  $i = 1, 2, \dots, m$ , on the loci located in the interval  $[a_i, a_{i+1})$ , the  $j$ th lineage carries ancestral materials of the sample sequences  $f_j(a_i)$ . The  $k$  ancestral lineages are kept unchanged until coalescence or recombination event happens. When a coalescence event happens, the algorithm chooses two lineages randomly from the  $k$  lineages and merges them into one lineage. When a recombination event happens, it draws a lineage randomly from the  $k$  lineages and splits it into two lineages with breakpoint  $s$ , whereas the breakpoint  $s \in (0, 1)$  is chosen according to a given distribution. The waiting times between two events are designed to be exponentially distributed with parameters depending on the current states. The algorithm starts at the present and performs back in time generating successive waiting times together with recombination or coalescence events. In Griffiths and Marjoram's program, the algorithm will repeat the above procedure until there is only one ancestral lineage, that is, until the GMRCA (grand most recent common ancestor) is found. To avoid redundant computation, *ms* algorithm has improved the above procedure in some aspects. In particular, *ms* respects the following two rules.

(R1) When the  $N$  samples have already found common ancestry in  $[0, u)$ , the algorithm will not perform any recombination event with breakpoint located in  $[0, u)$ .

(R2) A locus  $u$  in the sequence of a lineage can be chosen as a breakpoint only if both  $[0, u)$  and  $[u, 1)$  carry ancestral materials of the samples.

In this paper, we shall refer the algorithm with the above two rules as a *typical back-in-time algorithm*. (Remark: A minor difference between *ms* and our typical back-in-time algorithm is that in the above rule (R1), *ms* will respect common ancestry in  $[a, u)$  for any  $0 \leq a < u$ , while we respect only common ancestry in  $[a, u)$  with  $a = 0$ .) Since in the infinite allele model mutation is independent of the coalescent process with recombination, in our model we shall temporarily not consider mutation.

Below we shall show that  $E$  equipped with a suitable metric  $d$  is a locally compact separable space, which is crucial and very convenient for our further discussion.

Let  $x = \{f_1, f_2, \dots, f_k\} \in E$ . We say that  $s \in (0, 1)$  is a breakpoint of  $x$ , if there exist at least one  $f_j \in x$  such that  $f_j$  is discontinuous at  $s$ . Suppose that  $a_1 < a_2 < \dots < a_m$  are the different breakpoints of  $x$ . We make the convention that  $a_0 = 0$  and  $a_{m+1} = 1$ , then each  $f_j \in x$  may be expressed as  $f_j = \sum_{i=0}^m f_j(a_i) I_{[a_i, a_{i+1})}$ . We define

$$(2.2) \quad d_0(x) = \min_{0 \leq i \leq m} (a_{i+1} - a_i).$$

For  $m \geq 0$ , we set

$$(2.3) \quad V_m = \{x \in E : x \text{ has exactly } m \text{ different breakpoints}\}$$

and

$$(2.4) \quad V_m^* = \{x \in V_m : \text{all the breakpoints of } x \text{ are rational numbers}\}.$$

Let  $|x|$  be the number of elements in  $x$ . We set

$$(2.5) \quad U_k = \{x \in E : |x| = k\}.$$

PROPOSITION 1. (i) For  $f, h \in \mathcal{S}_{[0,1]}(\mathcal{P})$ , we define

$$d_L(f, h) = \int_0^1 d_p(f(s), h(s)) ds,$$

then  $d_L$  is a metric on  $\mathcal{S}_{[0,1]}(\mathcal{P})$ .

(ii) Let  $x, y \in E$ . Suppose that  $x = \{f_1, \dots, f_k\} \in V_m \cap U_k$  and  $y = \{h_1, \dots, h_l\} \in V_n \cap U_l$ , we define

$$(2.6) \quad d(x, y) = \max \left\{ \max_{1 \leq i \leq k} d_L(f_i, y), \max_{1 \leq j \leq l} d_L(h_j, x) \right\} + |k - l| + |m - n|$$

[ $d_L(f_i, y)$  stands for the distance from  $f_i$  to the set  $y$ ], then  $d$  is a metric on  $E$ .

The proof of Proposition 1 is presented in Section A.1 of the supplemental article [4].

For our purpose, we shall sometimes put the functions of a state  $x \in E$  in a parentheses to indicate that they have been well ranked in a specific order. More precisely, we may sometimes write  $x = (f_1, f_2, \dots, f_k)$ , which means that  $(f_1, f_2, \dots, f_k)$  have been ranked in such a way that if  $i < j$ , then either

$$(2.7) \quad \min\{s : f_i(s) \neq \emptyset\} < \min\{s : f_j(s) \neq \emptyset\}$$

or, in case that  $\min\{s : f_i(s) \neq \emptyset\} = \min\{s : f_j(s) \neq \emptyset\} =: S$ ,

$$(2.8) \quad \min f_i(S) < \min f_j(S).$$

Note that with the above specific order, the subscript “ $j$ ” of an element  $f_j \in x$  is uniquely determined.

The proposition below explores the neighborhood of a state  $x \in E$ .

**PROPOSITION 2.** *Let  $x = (f_1, f_2, \dots, f_k) \in V_m \cap U_k$  and  $a_1 < a_2 < \dots < a_m$  be the different breakpoints of  $x$ .*

(i) *Suppose that  $y \in E$  satisfies  $d(y, x) < 1$ , then  $y \in V_m \cap U_k$ .*

(ii) *Suppose that  $y = (h_1, h_2, \dots, h_k) \in E$  satisfies  $d(y, x) < \varepsilon \leq 3^{-1}d_0(x)$ . Let  $b_1 < b_2 < \dots < b_m$  be the different breakpoints of  $y$ . Then  $|b_i - a_i| < \varepsilon$  for all  $1 \leq i \leq m$ . Moreover, for each  $1 \leq j \leq k$ , it holds that  $d_L(h_j, f_j) = d_L(h_j, x) = d_L(y, f_j)$ , and  $h_j \in y$  can be expressed as*

$$(2.9) \quad h_j = \sum_{i=0}^m f_j(a_i) I_{[b_i, b_{i+1})}.$$

(iii) *For any  $\alpha > 0$  with  $\alpha < 3^{-1}d_0(x)$ , there exists an element  $y \in V_m^*$  such that  $d(y, x) < \alpha$ .*

The proof of Proposition 2 is presented in Section A.2 of the supplemental article [4].

Employing the above proposition, we can check the following topological properties of  $E$ .

**PROPOSITION 3.** (i) *For each  $m \geq 0$  and  $k \geq 1$ ,  $V_m \cap U_k$  is an isolated subset of  $E$ , that is,  $V_m \cap U_k$  is both open and closed in  $E$ .*

(ii)  *$E$  is a locally compact separable metric space.*

Proposition 3 is proved in Section A.2 of the supplemental article [4].

**2.2. Markov jump process.** In this subsection, we shall construct a Markov jump process describing the typical back-in-time algorithm. To formulate a rigorous mathematical model, we need to introduce some operations on  $\mathcal{S}_{[0,1)}(\mathcal{P})$  and on  $E$  corresponding to the algorithm.

Let  $f, h \in \mathcal{S}_{[0,1)}(\mathcal{P})$ . We define

$$(f \vee h)(s) := f(s) \cup h(s).$$

For  $u \in (0, 1)$ , we define

$$f^{(u-)}(s) := \begin{cases} f(s), & \text{if } s < u, \\ \emptyset, & \text{if } s \geq u, \end{cases}$$

$$f^{(u+)}(s) := \begin{cases} \emptyset, & \text{if } s < u, \\ f(s), & \text{if } s \geq u. \end{cases}$$



Then  $f \vee h, f^{(u-)}$  and  $f^{(u+)}$  are all elements of  $\mathcal{S}_{[0,1]}(\mathcal{P})$ .

For a state  $x = (f_1, f_2, \dots, f_k) \in E$ , we set

$$\begin{aligned} b_1(x) &= \inf\{u : f_1(u) \neq \{1, 2, \dots, N\}\}, \\ b_i(x) &= \inf\{u : f_i(u) \neq \emptyset\} \quad \forall 2 \leq i \leq k \end{aligned}$$

and

$$e_i(x) = \inf\{u : f_i(s) = \emptyset, \forall s \in (u, 1)\} \wedge 1 \quad \forall 1 \leq i \leq k.$$

We define for  $1 \leq i \leq k$  and  $u \in (b_i(x), e_i(x))$ ,

$$(2.10) \quad R_{iu}(x) = \{f_j : j \neq i\} \cup \{f_i^{(u-)}, f_i^{(u+)}\},$$

which indicates that a recombination event happens on the lineage  $f_i$  with breakpoint  $u$ . Note that the definitions of  $b_i$  and  $e_i$  ensure that the algorithm respects the above mentioned rule (R2). Moreover, the definition of  $b_1$ , which is different from the other  $b_i$ , and the ranking rule specified by (2.7) and (2.8) ensure that the algorithm respects the rule (R1). Further, we define for  $1 \leq i_1 < i_2 \leq k$ ,

$$(2.11) \quad C_{i_1, i_2}(x) = \{f_l : l \neq i_1, i_2\} \cup \{f_{i_1} \vee f_{i_2}\},$$

which denotes the coalescence of the lineages  $f_{i_1}$  and  $f_{i_2}$ .

We can now construct a Markov jump process  $\{X(t)\}$  as a rigorous mathematical model for our typical back-in-time algorithm. In what follows for any metric space  $E$ , we shall write  $\mathcal{B}(E)$  for the Borel subsets of  $E$ .

We define  $q(x, A)$  for  $x \in E$  and  $A \in \mathcal{B}(E)$  as follows:

$$(2.12) \quad q(x, A) := \sum_{1 \leq i_1 < i_2 \leq |x|} 1_A(C_{i_1, i_2}(x)) + \frac{\rho}{2} \sum_{i=1}^{|x|} \int_{b_i(x)}^{e_i(x)} p(s) I_A(R_{is}(x)) ds,$$

if  $|x| \geq 2$ , and

$$q(x, A) := 0 \quad \text{if } |x| = 1,$$

where  $I_A$  is the indicator function of  $A$ ,  $p(s)$  is the density function of a given distribution on  $(0, 1)$ , and  $\rho$  is a positive constant corresponding to a given recombination rate. Further, we define  $q(x)$  for  $x \in E$  by setting

$$(2.13) \quad q(x) := q(x, E).$$

For the terminologies involved in the proposition below, we refer to Definition 1.9 of [2].

**PROPOSITION 4.**  *$(q(x), q(x, A))$  defined by (2.13) and (2.12) is a  $q$ -pair in the sense that for each  $x \in E$ ,  $q(x, \cdot)$  is a measure on  $\mathcal{B}(E)$ ,  $q(x, \{x\}) = 0$ ,  $q(x, E) \leq q(x)$ ; and for each  $A \in \mathcal{B}(E)$ ,  $q(\cdot)$  and  $q(\cdot, A)$  are  $\mathcal{B}(E)$ -measurable. Moreover,  $(q(x), q(x, A))$  is totally stable in the sense that  $0 \leq q(x) < \infty$  for all  $x \in E$ , and is conservative in the sense that  $q(x) = q(x, E)$  for all  $x \in E$ .*



The proof of Proposition 4 is presented in Section A.3 of the supplemental article [4].

By virtue of Proposition 4 and making use of the theory of  $q$ -processes we obtain the following proposition.

**PROPOSITION 5.** *Given any initial distribution  $\mu$  on  $\mathcal{B}(E)$ , there exists a  $q$ -process  $\{X(t), t \geq 0\}$  corresponding to the  $q$ -pair  $(q(x), q(x, A))$ , in the sense that  $\{X(t)\}$  is a time homogeneous Markov jump process satisfying: (i)  $P\{X(0) \in A\} = \mu(A)$ ; (ii) the transition probability of its embedded Markov chain is given by*

$$(2.14) \quad \Pi(x, A) = I_{\{q(x) \neq 0\}} \frac{q(x, A)}{q(x)} + I_{\{q(x) = 0\}} I_A(x);$$

(iii) the waiting time of its jump given  $X(t) = x$  is exponentially distributed with parameter  $q(x)$ .

The proof of Proposition 5 is presented in Section A.4 of the supplemental article [4].

Define

$$(2.15) \quad \Delta := \{f\} \quad \text{with } f = \{1, 2, \dots, N\} I_{[0,1]}.$$

Note that  $\Delta$  is the only element in  $U_1 := \{x \in E : |x| = 1\}$ , and hence is the only absorbing state in  $E$  satisfying  $q(x, E) = 0$ .

**PROPOSITION 6.** *The transition semigroup of the  $q$ -process specified by Proposition 5 is unique. Moreover, the process will almost surely arrive at the absorbing state  $\Delta$  in at most finitely many jumps.*

The proof of Proposition 6 is presented in Section A.5 of the supplemental article [4].

**2.3. ARG space  $G$ .** Let  $\{X(t), t \geq 0\}$  be the Markov jump process constructed in Proposition 5 with initial distribution  $\delta_{\{\varpi\}}$ , where  $\varpi$  is specified by (2.1). Assume that  $\{X(t)\}$  is defined on some probability space  $(\Omega, \mathcal{F}, P)$ . Then for each  $\omega \in \Omega$ ,  $X(\cdot)(\omega)$  is an element in  $\mathcal{S}_{[0,\infty)}(E)$ , where  $\mathcal{S}_{[0,\infty)}(E)$  denotes the family of all the  $E$ -valued right continuous piecewise constant functions on  $[0, \infty)$  with at most finitely many discontinuity points. Note that not all elements  $g \in \mathcal{S}_{[0,\infty)}(E)$  can be regarded as an ARG generated by the back-in-time algorithm. Indeed, if  $g \in \mathcal{S}_{[0,\infty)}(E)$  represents an ARG, then  $g = \{g(t), t \geq 0\}$  should satisfy the following two intuitive requirements. (i)  $g(0) = \varpi$  and if  $g(t) \neq g(t_-)$ , then  $g(t)$  is generated by a coalescent event or a recombination event from the state  $g(t_-) \in E$ . (ii) Along the path  $\{g(t), t \geq 0\}$ , recombination events will not happen more than once in any

locus  $s \in (0, 1)$ . Below we shall prove that with probability one,  $\{X(t), t \geq 0\}$  satisfies the above two requirements, and hence represents an ARG. To state our result rigorously, we introduce some notation first.

For a state  $x = (f_1, \dots, f_k) \in E$  with  $|x| \geq 2$ , we set

$$(2.16) \quad \begin{aligned} E_x &= \{C_{i_1, i_2}(x) : 1 \leq i_1 < i_2 \leq |x|\} \\ &\cup \{R_{is}(x) : 1 \leq i \leq |x|, s \in (b_i(x), e_i(x))\}. \end{aligned}$$

For notational convenience, we shall also write  $x = E_x$  if  $x \in E$  with  $|x| = 1$ . We define a function  $\mathcal{U} : E \times E \rightarrow (0, 1) \cup \{-1\}$  by setting

$$(2.17) \quad \begin{aligned} (x, y) &\rightarrow \mathcal{U}(x, y) \\ &= \begin{cases} u, & \text{if there exists a unique } u \in (0, 1) \\ & \text{such that } y = R_{iu}(x) \text{ for some } 1 \leq i \leq k; \\ -1, & \text{else.} \end{cases} \end{aligned}$$

We set for  $g \in \mathcal{S}_{[0, \infty)}(E)$ ,

$$(2.18) \quad \tau_0 \equiv 0, \quad \tau_n := \tau_n(g) = \inf\{t > \tau_{n-1} : g(t) \neq g(\tau_{n-1})\} \quad \forall n \geq 1,$$

with the convention that  $\inf \emptyset = \infty$  and  $g(\infty) = \Delta$ . For the sake of convenience, we shall write  $\mathcal{U}_n(g) := \mathcal{U}(g(\tau_{n-1}), g(\tau_n))$ . We define

$$(2.19) \quad G' := \{g \in \mathcal{S}_{[0, \infty)}(E) : g(\tau_0) = \varpi \text{ and } g(\tau_n) \in E_{g(\tau_{n-1})} \text{ for all } n \geq 1\}$$

and

$$(2.20) \quad G := \{g \in G' : \mathcal{U}_n(g) \neq \mathcal{U}_j(g) \text{ for all } n \neq j \text{ whenever } \mathcal{U}_j(g) \in (0, 1)\}.$$

It is easy to see that if  $g \in G$ , then  $g$  satisfies the above two intuitive requirements. We shall call  $G$  the *ARG space*.

**PROPOSITION 7.** *There exists  $\Omega_0 \in \mathcal{F}$  with  $P(\Omega_0) = 1$ , such that for all  $\omega \in \Omega_0$ , we have  $X(\cdot)(\omega) \in G$ .*

The proof of Proposition 7 is presented in Section A.6 of the supplemental article [4].

Note that the ARG space  $G$  specified by (2.20) is a subset of the  $E$ -valued Skorohod space  $D_E[0, \infty)$ . We are going to show that  $G$  equipped with the Skorohod topology is a locally compact separable metric space.

We first introduce some terminologies and notation. For  $g \in G$ , we set  $\gamma(g) = \inf\{n : \tau_{n+1}(g) = \infty\}$  where  $\tau_n(g)$  is defined by (2.18). Let  $Bp(g) := Bp(g(\tau_0), g(\tau_1), \dots, g(\tau_{\gamma(g)}))$  be the collection of all the breakpoints on  $g$ . Then  $Bp(g)$  consists of at most finitely many points of  $(0, 1)$ . Moreover, by (2.20) the points of  $Bp(g)$  are all different from each other. Denote by  $|Bp(g)|$  the number of points contained in  $Bp(g)$ . We define  $S_i := S_i(g)$  to be the  $i$ th

order statistic of  $Bp(g)$ . That is,  $Bp(g) = \{S_1, S_2, \dots, S_{|Bp(g)|}\}$  and  $S_i < S_{i+1}$  for all  $i$ . For convenience, we make the convention that  $S_0 = 0$  and  $S_i = 1$  for  $i > |Bp(g)|$ . Suppose that  $|Bp(g)| = m$  and  $g(t) = \{f_1, f_2, \dots, f_{|g(t)|}\} \in E$ , we define an  $(m+1)$ -dimensional  $\mathcal{P}$ -valued vector for each  $f_j \in g(t)$  by setting  $\mathfrak{S}_j(g(t)) := (f_j(S_0), f_j(S_1), \dots, f_j(S_m))$ . Further, we write  $\mathfrak{S}(g(t)) = \{\mathfrak{S}_j(g(t)) : 1 \leq j \leq |g(t)|\}$ . It is clear that  $\mathfrak{S}(g(t)) = \mathfrak{S}(g(\tau_n))$  when  $\tau_n \leq t < \tau_{n+1}$  for all  $n$ . In what follows, we set  $d_0(g) = \min_{0 \leq i \leq |Bp(g)|} (S_{i+1}(g) - S_i(g))$ .

For the convenience of the reader, we recall the definition of the Skorohod metric  $d_S$  on  $D_E[0, \infty)$  (cf. [6]).

Let  $\Lambda$  be the collection of Lipschitz continuous and strictly increasing functions  $\lambda$  such that  $\kappa(\lambda) := \sup_{s>t \geq 0} |\log \frac{\lambda(s) - \lambda(t)}{s - t}| < \infty$ . For  $g_1, g_2 \in D_E[0, \infty)$ , the Skorohod metric  $d_S$  is defined as

$$(2.21) \quad d_S(g_1, g_2) = \inf_{\lambda \in \Lambda} \left[ \kappa(\lambda) \vee \int_0^\infty e^{-u} d(g_1, g_2, \lambda, u) du \right],$$

where

$$d(g_1, g_2, \lambda, u) = \sup_{t \geq 0} d(g_1(t \wedge u), g_2(\lambda(t) \wedge u)) \wedge 1.$$

The proposition below plays an important role in our further study.

**PROPOSITION 8.** *Let  $g_l, g_0 \in G$ . Suppose that*

$$(2.22) \quad d_S(g_l, g_0) < 3^{-1} d_0(g_0) e^{-2\tau_{\gamma(g_0)}(g_0)}.$$

*Then the following assertions hold:*

- (i)  $\gamma(g_l) = \gamma(g_0)$ .
- (ii)  $|Bp(g_l)| = |Bp(g_0)|$  and  $\mathfrak{S}(g_l(\tau_n)) = \mathfrak{S}(g_0(\tau_n))$  for all  $1 \leq n \leq \gamma(g_0)$ .
- (iii)  $d(g_l(\tau_n), g_0(\tau_n)) \leq e^{2\tau_{\gamma(g_0)}(g_0)} d_S(g_l, g_0) < 3^{-1} d_0(g_0)$  for all  $1 \leq n \leq \gamma(g_0)$ .

Proposition 8 is proved in Section A.7 of the supplemental article [4].

**PROPOSITION 9.** (i) *Let  $\{g_l, l \geq 1\} \subset G$  and  $g_0 \in G$ . Then  $\lim_{l \rightarrow \infty} d_S(g_l, g_0) = 0$  if and only if  $S_i(g_l) \rightarrow S_i(g_0)$  for all  $i \geq 1$ ,  $\tau_n(g_l) \rightarrow \tau_n(g_0)$  for all  $n \geq 1$ , and there exists  $l_0$  such that for all  $l \geq l_0$  the assertions of Proposition 8(i)–(iii) hold.*

(ii)  *$G$  equipped with the Skorohod metric  $d_S$  is a locally compact separable metric space.*

The proof of Proposition 9 is presented in Section A.8 of the supplemental article [4].

Note that  $G$  can be regarded as the collection of all the ARGs generated by the back-in-time algorithm. We denote by  $\mathcal{B}(G)$  the Borel sets of  $G$ .

**THEOREM 1.** *Let  $P$  be the probability distribution on  $(G, \mathcal{B}(G))$  generated by the typical back-in-time algorithm, and denote by  $\{X(t), t \geq 0\}$  the coordinate process on  $G$ . Then  $\{X(t), t \geq 0\}$  is an  $E$ -valued Markov jump process corresponding to the  $q$ -pair (2.12)–(2.13).*

**PROOF.** Since on the Skorohod space the Borel  $\sigma$ -field coincides with the  $\sigma$ -field generated by its coordinate process (cf., e.g., [6]), the theorem follows directly from Propositions 7 and 9(ii).  $\square$

Before concluding this subsection, we explore some properties of  $Bp(g)$  and  $\mathfrak{S}(g(t))$  as stated in Proposition 10 below, which will play an important role in our further discussion.

Below we denote by  $\mathcal{P}^{m+1}$  the totality of  $(m+1)$ -dimensional  $\mathcal{P}$ -valued vectors. For  $\vec{z} = (z_0, z_1, \dots, z_m) \in \mathcal{P}^{m+1}$ , we define  $\pi_j(\vec{z}) = z_j$  for  $0 \leq j \leq m$ . For  $\vec{a} = (a_0, a_1, \dots, a_m) \in \mathcal{P}^{m+1}$  and  $\vec{b} = (b_0, b_1, \dots, b_m) \in \mathcal{P}^{m+1}$ , we define  $\vec{a} \vee \vec{b} \in \mathcal{P}^{m+1}$  by setting  $\pi_j(\vec{a} \vee \vec{b}) = a_j \cup b_j$ . Further, for  $1 \leq j \leq m$ , we define  $(\vec{a})^{j-} \in \mathcal{P}^{m+1}$  by setting  $\pi_i((\vec{a})^{j-}) = a_i$  for  $i < j$  and  $\pi_i((\vec{a})^{j-}) = \emptyset$  for  $i \geq j$ , define  $(\vec{a})^{j+} \in \mathcal{P}^{m+1}$  by setting  $\pi_i((\vec{a})^{j+}) = \emptyset$  for  $i < j$  and  $\pi_i((\vec{a})^{j+}) = a_i$  for  $i \geq j$ . We say that a vector  $\vec{z} \in \mathcal{P}^{m+1}$  is null, if  $\pi_j(\vec{z}) = \emptyset$  for all  $0 \leq j \leq m$ .

**PROPOSITION 10.** *For  $g \in G$  with  $|Bp(g)| = m$  and  $\gamma(g) = \gamma$ , we denote by  $S_i = S_i(g)$  the  $i$ th order statistic of  $Bp(g)$  for  $1 \leq i \leq m$ , and write  $\mathfrak{S}(t)$  for  $\mathfrak{S}(g(t))$ . Then the following assertions hold:*

- (i) *For all  $t$ ,  $\mathfrak{S}(t)$  is a finite subset of  $\mathcal{P}^{m+1}$  such that  $\{\pi_i(\vec{z}) : \vec{z} \in \mathfrak{S}(t), \pi_i(\vec{z}) \neq \emptyset\}$  form a partition of  $\{1, 2, \dots, N\}$  for each  $0 \leq i \leq m$ . Moreover, any  $\vec{z} \in \mathfrak{S}(t)$  is not null.*
- (ii) *There exist  $\{\tau_n : 1 \leq n \leq \gamma\}$  with  $\tau_0 := 0 < \tau_1 < \tau_2 < \dots < \tau_\gamma < \infty := \tau_{\gamma+1}$  such that  $\mathfrak{S}(\tau_n) \neq \mathfrak{S}(\tau_{n+1})$  and  $\mathfrak{S}(t) = \mathfrak{S}(\tau_n)$  when  $t \in [\tau_n, \tau_{n+1})$  for all  $0 \leq n \leq \gamma$ .*
- (iii) *For  $1 \leq n \leq \gamma$ , if we write  $\mathfrak{S}(\tau_{n-1}) = \{\vec{z}_1, \vec{z}_2, \dots, \vec{z}_k\}$ . Then either  $\mathfrak{S}(\tau_n) = \{\vec{z}_l : l \neq j_1, j_2\} \cup \{\vec{z}_{j_1} \vee \vec{z}_{j_2}\}$  for some  $1 \leq j_1 < j_2 \leq k$ , or  $\mathfrak{S}(\tau_n) = \{\vec{z}_l : l \neq j\} \cup \{(\vec{z}_j)^{i-}, (\vec{z}_j)^{i+}\}$  for some  $1 \leq j \leq k$  and some  $1 \leq i \leq m$ .*
- (iv) *For each  $1 \leq i \leq m$ , there exists  $\tau_{n(i)} \in \{\tau_1, \tau_2, \dots, \tau_\gamma\}$  at which  $S_i$  appears in the following sense: if we write  $\mathfrak{S}(\tau_{n(i)-1}) = \{\vec{z}_1, \vec{z}_2, \dots, \vec{z}_k\}$ , then  $\mathfrak{S}(\tau_{n(i)}) = \{\vec{z}_l : l \neq j\} \cup \{(\vec{z}_j)^{i-}, (\vec{z}_j)^{i+}\}$  for some  $\vec{z}_j \in \mathfrak{S}(\tau_{n(i)-1})$  satisfying  $\pi_{i-1}(\vec{z}_j) = \pi_i(\vec{z}_j) \neq \emptyset$ . Moreover, the time point  $\tau_{n(i)}$  at which  $S_i$  appears is unique.*
- (v) *For  $t \in [\tau_n, \tau_{n+1})$ , if we write  $\mathfrak{S}(\tau_n) = \{\vec{z}_1, \vec{z}_2, \dots, \vec{z}_k\}$  and make the convention that  $S_0 = 0$  and  $S_{m+1} = 1$ , then  $g(t)$  is expressed as  $g(t) = \{f_1, f_2, \dots, f_k\}$  with  $f_j = \sum_{l=0}^m \pi_l(\vec{z}_j) I_{[S_l, S_{l+1})}$  for each  $1 \leq j \leq k$ .*

**PROOF.** All the assertions can be checked directly by the definition of  $Bp(g)$  and  $\mathfrak{S}(g(t))$ , as well as Definition 1, (2.19) and (2.20), we leave the details to the reader.  $\square$

### 3. Main results: Spatially moving model.

3.1. *Random sequence*  $\{(S_i, Z^i), i \geq 0\}$ . Let  $(G, \mathcal{B}(G), P)$  be the probability space specified in Theorem 1. In this subsection, we shall define a sequence of random variables  $\{(S_i, Z^i), i \geq 0\}$  on  $(G, \mathcal{B}(G), P)$  and derive their distributions, which will be used to model our spatial algorithm.

3.1.1. *Definition and structure of*  $\{(S_i, Z^i), i \geq 0\}$ . In Section 2.3, we have defined  $S_i := S_i(g)$  to be the  $i$ th order statistic of  $Bp(g)$ . With the convention that  $S_0 = 0$  and  $S_i = 1$  for  $i > |Bp(g)|$ , by Proposition 9 we see that  $\{S_i, i \geq 0\}$  is a sequence of continuous mappings from  $G$  to  $[0, 1]$ . In what follows, we define the random sequence  $\{Z^i, i \geq 0\}$ .

Below for  $\vec{z} = (z_0, z_1, \dots, z_m) \in \mathcal{P}^{m+1}$  and  $0 \leq i < m$ , we write  $\pi_{[0,i]}(\vec{z}) = (z_0, \dots, z_i)$ . For a subset  $A \subset \mathcal{P}^{m+1}$ , we write  $\pi_{[0,i]}^*(A) := \{\pi_{[0,i]}(\vec{a}) : \vec{a} \in A, \pi_{[0,i]}(\vec{a}) \text{ is not null in } \mathcal{P}^{i+1}\}$  for  $i < m$ , and make the convention that  $\pi_{[0,i]}^*(A) = A$  for  $i \geq m$ . Let  $g \in G$ . For  $i = 0$ , we define

$$(3.1) \quad T_0^0 = 0, \quad Z^0(t) := Z^0(t)(g) = \pi_{[0,0]}^*(\mathfrak{S}(g(t))).$$

For  $1 \leq i \leq |Bp(g)|$ , we set

$$(3.2) \quad \xi^i := \xi^i(g) = \pi_i(\vec{z}_j),$$

where  $\pi_i(\vec{z}_j)$  is specified in Proposition 10(iv), that is,  $\xi^i$  is the type set involved at the recombination at locus  $S_i$  when it first becomes a breakpoint. Further, we define

$$(3.3) \quad T_0^i := T_0^i(g) = \tau_{n(i)}, \quad Z^i(t) := Z^i(t)(g) = \pi_{[0,i]}(\vec{z}_l) \quad \text{for } t \geq T_0^i,$$

here  $\tau_{n(i)}$  is specified in Proposition 10(iv) and  $\vec{z}_l$  is the unique vector in  $\mathfrak{S}(g(t))$  satisfying  $\pi_i(\vec{z}_l) \supseteq \xi^i$ . Note that the existence and uniqueness of  $\vec{z}_l$  employed above is ensured by Proposition 10(i). Intuitively,  $Z^i(t)$  traces those lineages containing the genotypes  $\xi^i$  at locus  $S_i$ , the ancestral materials  $\vec{z}_l$  and  $\vec{z}_j$  are objects at different times  $t$  and  $\tau_{n(i)-1}$ , respectively. For  $i > |Bp(g)|$ , we make the convention that  $T_0^i = \infty$  and  $Z^i(t) \equiv \vec{\emptyset}$ , here  $\vec{\emptyset}$  denotes the null vector in  $\mathcal{P}^{i+1}$ .

For each  $i \geq 1$ , we define recursively for  $n \geq 1$ ,

$$(3.4) \quad T_n^i = \inf\{t > T_{n-1}^i : Z^i(t) \neq Z^i(T_{n-1}^i)\}$$

and

$$(3.5) \quad \xi_n^i = Z^i(T_n^i),$$

with the convention that  $Z^i(\infty) = \vec{\emptyset}$ . For convenience, we make the further convention that  $Z^i(t) = \vec{\emptyset}$  when  $t < T_0^i$ . Then  $\{Z^i(t), t \geq 0\}$  is uniquely determined by the  $(\overline{R}^+ \times \mathcal{P}^{i+1})$ -valued sequence  $\{(T_n^i, \xi_n^i) : n \geq 0\}$ . (Here and

henceforth,  $\overline{R}^+ := [0, \infty]$ .) We remind the reader that for  $1 \leq i \leq |Bp(g)|$ , we have  $\xi_0^i = (\emptyset, \dots, \emptyset, \xi^i)$  where  $\xi^i$  was used as a label for defining  $Z^i(t)$  [cf. (3.2), (3.3)]. Below we endow the product topology on  $\overline{R}^+ \times \mathcal{P}^{i+1}$ .

PROPOSITION 11. (i) For each  $i$  and  $n$ ,  $(T_n^i, \xi_n^i)$  is a continuous functional from  $G$  to  $\overline{R}^+ \times \mathcal{P}^{i+1}$ .

(ii) For each  $i$ ,  $\{Z^i(t), t \geq 0\}$  is a jump process on  $G$  with at most finitely many jumps.

Proposition 11 is proved in Section A.9 of the supplemental article [4].

We now study the measurable structure of  $\{(S_i, Z^i), i \geq 0\}$ . Let  $g \in G$ . We define for  $i = 0$ ,

$$(3.6) \quad V(Z^0; t) = Z^0(t)(g).$$

For  $1 \leq i \leq Bp(g)$ , we define  $V(Z^0, Z^1, \dots, Z^i; t) := V(Z^0, Z^1, \dots, Z^i; t)(g)$  recursively by the scheme below. For  $t < T_0^i$ , define

$$(3.7) \quad \begin{aligned} & V(Z^0, Z^1, \dots, Z^i; t) \\ &= \{\vec{z} \in \mathcal{P}^{i+1} : \pi_{[0, i-1]}(\vec{z}) \in V(Z^0, Z^1, \dots, Z^{i-1}; t), \pi_i(\vec{z}) = \pi_{i-1}(\vec{z})\}; \end{aligned}$$

for  $t \geq T_0^i$ , define

$$(3.8) \quad \begin{aligned} & V(Z^0, Z^1, \dots, Z^i; t) \\ &= \{Z^i(t)\} \\ & \cup \{\vec{z} \in \mathcal{P}^{i+1} : \pi_{[0, i-1]}(\vec{z}) \in V(Z^0, Z^1, \dots, Z^{i-1}; t) \setminus \{\pi_{[0, i-1]}(Z^i(t))\}, \\ & \quad \pi_i(\vec{z}) = \pi_{i-1}(\vec{z}) \setminus \xi^i\}. \end{aligned}$$

For  $i > Bp(g)$ , we define  $V(Z^0, Z^1, \dots, Z^i; t) = \mathfrak{S}(g(t))$ .

PROPOSITION 12. Let  $V(Z^0, Z^1, \dots, Z^i; t) := V(Z^0, Z^1, \dots, Z^i; t)(g)$  be defined as above. Then for each  $i \geq 0$ , we have

$$(3.9) \quad V(Z^0, Z^1, \dots, Z^i; t) = \pi_{[0, i]}^*(\mathfrak{S}(g(t))).$$

Proposition 12 is proved in Section A.10 of the supplemental article [4].

Next, for  $s \in [0, 1)$  and  $f \in \mathcal{S}_{[0, 1)}(\mathcal{P})$ , we define  $f^s \in \mathcal{S}_{[0, 1)}(\mathcal{P})$  by setting

$$f^s(u) := \begin{cases} f(u), & \text{if } u < s, \\ f(s), & \text{if } u \geq s. \end{cases}$$

For  $x = \{f_1, f_2, \dots, f_k\} \in E$ , we define  $\pi_{[0, s]}^E(x) \in E$  by setting

$$(3.10) \quad \pi_{[0, s]}^E(x) := \{f_j^s : 1 \leq j \leq k, f_j^s \neq \emptyset\}.$$

Applying Proposition 2(ii), one can check that  $\pi_{[0,s]}^E$  is a measurable map from  $(E, \mathcal{B}(E))$  to  $(E, \mathcal{B}(E))$ . Below we shall sometimes write  $x^s = \pi_{[0,s]}^E(x)$ , and write  $[x^s] = (\pi_{[0,s]}^E)^{-1}\{x^s\} =: \{y \in E : y^s = x^s\}$ . Let  $\sigma(\pi_{[0,s]}^E)$  be the sub  $\sigma$ -algebra of  $\mathcal{B}(E)$  generated by  $\pi_{[0,s]}^E$ . Then  $[x^s]$  is an atom of  $\sigma(\pi_{[0,s]}^E)$  for each  $x \in E$ .

For  $g \in G$ , we define  $\pi_{[0,s]}^G(g)$  by setting

$$(3.11) \quad \pi_{[0,s]}^G(g)(t) := \pi_{[0,s]}^E(g(t)) \quad \forall t \geq 0.$$

PROPOSITION 13.  $\pi_{[0,s]}^G$  is a measurable map from  $(G, \mathcal{B}(G))$  to  $(G, \mathcal{B}(G))$ .

Proposition 13 is proved in Section A.11 of the supplemental article [4].

We extend the definition of  $\pi_{[0,s]}^G(g)$  by setting  $\pi_{[0,s]}^G(g) = g$  for  $s \geq 1$ . Write  $X^s(g) := \pi_{[0,s]}^G(g)$ . Then  $\{X^s, s \geq 0\}$  can be viewed as a  $G$ -valued stochastic process defined on the probability space  $(G, \mathcal{B}(G), P)$ . From Proposition 10(v), we see that  $\{X^s\}$  is a jump process, that is, its paths are piecewise constant and right continuous with left limits. Define  $S'_0 = 0$  and  $S'_i = \inf\{t > S'_{i-1} : X^t \neq X^{S'_{i-1}}\}$  for  $i \geq 1$ . That is,  $S'_i$  is the  $i$ th jump time of  $\{X^s\}$ . Let  $\mathcal{F}^s = \sigma(X^u, u \leq s)$ ,  $s \geq 0$ , be the natural filtration of  $\{X^s\}$  and  $\mathcal{F}^\infty = \bigvee_{s \geq 0} \mathcal{F}^s$ . Since for  $0 < u \leq s$ , it holds that  $X^u = \pi_{[0,u]}^G(X^s)$ , therefore,  $X^u$  is  $\sigma(X^s)$  measurable. Thus,  $\mathcal{F}^s = \sigma(X^s)$  and  $\{X^s, s \geq 0\}$  is a  $G$ -valued Markov process with respect to its natural filtration. The proposition below shows that  $\{(S_i, Z^i), i \geq 0\}$  enjoys a very nice measurable structure.

PROPOSITION 14. For  $i \geq 1$ , we have

$$\sigma(S_1, \dots, S_i; Z^0, Z^1, \dots, Z^i) = \sigma(X^{S_i}) = \sigma(X^0, S_1, \dots, S_i; X^{S_1}, \dots, X^{S_i}).$$

Proposition 14 is proved in Section 4.1.

3.1.2. *Distribution of  $S_i$ .* We write  $\pi_t(g) = g(t)$  for  $g \in G \subset D_E[0, \infty)$ . For fixed  $s \geq 0$ , we write  $X^s(t)(g) = \pi_t(X^s(g))$ . It is easy to see that  $X^s(t) = X(t)^s := \pi_{[0,s]}^E(X(t))$ . Therefore,  $\{X^s(t)(\cdot), t \geq 0\}$  is a jump process taking values in  $(E^s, \mathcal{B}(E^s))$ . Here and henceforth,

$$(3.12) \quad E^s := \pi_{[0,s]}^E(E) = \{x^s : x \in E\}.$$

Note that  $E^s = \{x \in E : x = \pi_{[0,s]}^E(x)\}$ , hence  $E^s$  is a Borel subset of  $E$ .

Set  $\tau_0^s = 0$  and for  $n \geq 1$  define

$$(3.13) \quad \tau_n^s = \inf\{t > \tau_{n-1}^s : X^s(t) \neq X^s(\tau_{n-1}^s)\}.$$



Since  $\mathcal{B}(G) = G \cap \mathcal{B}(D_E[0, \infty)) = G \cap \sigma\{\pi_t^{-1}(B) : B \in \mathcal{B}(E), t \geq 0\}$ , we have that

$$(3.14) \quad \begin{aligned} \mathcal{F}^s &= \sigma(X^s) = \sigma\{X^s(t) : t \geq 0\} \\ &= \sigma\{X^s(0), \tau_1^s, X^s(\tau_1^s), \tau_2^s, X^s(\tau_2^s), \dots\}. \end{aligned}$$

The proposition below is crucial for deriving the distributions of  $\{(S_i, Z^i) : i \geq 0\}$ . Its proof is quite long and involves a study of projections of q-processes. To avoid digression from the main topics of this paper, the proof will appear elsewhere. In what follows, we always assume that  $y_0 = \varpi$  where  $\varpi$  was specified by (2.1).

**PROPOSITION 15.** *Let  $0 \leq u \leq s \leq 1$ . For  $n \geq 1$  and  $k \geq 0$ , we define  $\vartheta_j := \tau_n^s + \tau_{j-n}^u \circ \theta_{\tau_n^s}$  for  $n \leq j \leq n+k$ , where  $\theta_{\tau_n^s}$  is the time shift operator with respect to the  $(\mathcal{F}_t)$ -stopping time  $\tau_n^s$  ( $(\mathcal{F}_t)_{t \geq 0}$  refers to the natural filtration generated by  $\{X(t), t \geq 0\}$ ). Then for  $B \in \mathcal{B}((R^+ \times E)^{n+k})$ , we have*

$$\begin{aligned} &P\{(\tau_1^s, X^s(\tau_1^s), \dots, \tau_n^s, X^s(\tau_n^s), \vartheta_{n+1}, X^u(\vartheta_{n+1}), \dots, \vartheta_{n+k}, X^u(\vartheta_{n+k}) \in B)\} \\ &= \int_0^\infty dt_1 \cdots \int_0^\infty dt_{n+k} \int_E q(y_0, dy_1) \cdots \\ &\quad \int_E q(y_{n-1}, dy_n) \int_E q(\pi_{[0,u]}^E(y_n), dy_{n+1}) \\ &\quad \int_E q(y_{n+1}, dy_{n+2}) \cdots \int_E q(y_{n+k-1}, dy_{n+k}) I_B(t_1, y_1, \dots, t_{n+k}, y_{n+k}) \\ &\quad \cdot I_{\{t_1 < \dots < t_{n+k}\}}(t_1, \dots, t_{n+k}) \prod_{j=0}^{n-1} I_{E^s}(y_{j+1}) \prod_{i=0}^{k-1} I_{E^u}(y_{n+i+1}) \\ &\quad \cdot \exp \left\{ - \sum_{j=0}^{n-1} q(y_j, [y_j^s]^c)(t_{j+1} - t_j) \right. \\ &\quad \left. - \sum_{i=0}^{k-1} q(y_{n+i}, [y_{n+i}^u]^c)(t_{n+i+1} - t_{n+i}) \right\}. \end{aligned}$$

**PROOF.** See [3].  $\square$

For  $x = \{f_1, f_2, \dots, f_k\} \in E$ , we define  $\pi_s^E(x) \subset \mathcal{P}$  by setting

$$(3.15) \quad \pi_s^E(x) := \{f_j(s) : f_j(s) \neq \emptyset, j = 1, 2, \dots, k\}.$$

Note that by Definition 1,  $\pi_s^E(x)$  is a partition of  $\{1, 2, \dots, N\}$ . For  $g \in G$ ,  $s \in [0, 1)$ , we write

$$(3.16) \quad \mathcal{T}_s(t)(g) = \pi_s^E(g(t)) \quad \text{and} \quad L_s(g) = \int_0^{\beta_s} |\mathcal{T}_s(t)(g)| dt,$$

where  $\beta_s = \inf\{t : |X^s(t)(g)| = 1\}$ . Intuitively,  $\{\mathcal{T}_s(t), t \geq 0\}$  is the coalescent tree at site  $s$ , and  $L_s(g)$  is the total length of the coalescent tree  $\mathcal{T}_s(g)$  before  $\beta_s$ .

**THEOREM 2.** *For  $i \geq 0$ , the distribution of  $S_{i+1}$  conditioning on  $\mathcal{F}^{S_i}$  is: for  $s < 1$ ,*

$$P(S_{i+1} > s | \mathcal{F}^{S_i}) = \exp \left\{ -\rho L_{S_i}(X^{S_i}) \int_{S_i}^{s \vee S_i} 2^{-1} p(r) dr \right\}$$

and

$$P(S_{i+1} = 1 | \mathcal{F}^{S_i}) = \exp \left\{ -\rho L_{S_i}(X^{S_i}) \int_{S_i}^1 2^{-1} p(r) dr \right\}.$$

Theorem 2 is proved in Section 4.2.

### 3.1.3. Distribution of $Z^i$ .

**THEOREM 3.** *We have  $Z^0(t) = \mathcal{T}_0(t)$ , and the distribution of  $\mathcal{T}_0 = \{\mathcal{T}_0(t), t \geq 0\}$  follows that of a standard Kingman's coalescent tree developed in [12].*

Theorem 3 is proved in Section 4.3.

Below we study the distribution of  $Z^{i+1}$  conditioning on  $\mathcal{F}^{S_i} \vee \sigma(S_{i+1})$  for each  $i \geq 0$ . Note that for  $i \geq 1$ ,  $\{Z^i(t), t \geq 0\}$  is uniquely determined by the  $(\bar{R}^+ \times \mathcal{P}^{i+1})$ -valued sequence  $\{(T_n^i, \xi_n^i) : n \geq 0\}$ . Thus, by virtue of Proposition 14, we need only to calculate the distribution of  $\{(T_n^{i+1}, \xi_n^{i+1}) : n \geq 0\}$  conditioning on  $\sigma(X^{S_i}, S_{i+1})$ .

Let  $i \geq 0$  be fixed. We calculate first  $P(T_0^{i+1} \leq t, \xi^{i+1} = \xi | X^{S_i}, S_{i+1})$  for  $t \geq 0, \xi \in \mathcal{P}$ . The theorem below shows that the location where  $S_{i+1}$  first appears is uniformly distributed on  $\mathcal{T}_{S_i}$ .

**THEOREM 4.** *For any  $t \geq 0, \xi \in \mathcal{P}$ , we have*

$$P(T_0^{i+1} \leq t, \xi^{i+1} = \xi | X^{S_i}, S_{i+1}) = \lambda(\{u : u \leq t, u < \beta_{S_i}, \xi \in \mathcal{T}_{S_i}(u)\}) / L_{S_i},$$

where  $\lambda$  is the Lebesgue measure and  $\beta_{S_i} := \inf\{t : |X^{S_i}| = 1\}$ .

Theorem 4 is proved in Section 4.4.

For fixed  $j \geq 0$ , with much more complicated argument and discussion, we can calculate the conditional distribution  $P(T_{j+1}^{i+1} \in B, \xi_{j+1}^{i+1} = \vec{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1})$  for arbitrary  $B \in \mathcal{B}(R^+)$  and  $\vec{\xi} \in \mathcal{P}^{i+2}$ . The detailed discussion is given in the supplemental article [4]. The corresponding results are divided into 3 cases and stated below.

*Case 1:*  $\xi_j^{i+1} = \xi_0^{i+1}$ . Since  $\pi_{[0,i]}(\xi_0^{i+1}) = \vec{\emptyset}$ , and the time point at which  $S_{i+1}$  appears is unique [cf. Proposition 10(iv)], in this case the next event at time point  $T_{j+1}^{i+1}$  must be a coalescence. We have the following theorem.

THEOREM 5. Suppose that  $\xi_j^{i+1} = \xi_0^{i+1}$ .

(i) For  $\vec{\xi} \in \mathcal{P}^{i+2}$  satisfying  $\pi_{i+1}(\vec{\xi}) \neq \pi_{i+1}(\xi_0^{i+1}) \cup \pi_i(\vec{\xi})$ , we have

$$P(\xi_{j+1}^{i+1} = \vec{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi_0^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1}) = 0.$$

(ii) For  $\vec{\xi} \in \mathcal{P}^{i+2}$  satisfying  $\pi_{i+1}(\vec{\xi}) = \pi_{i+1}(\xi_0^{i+1}) \cup \pi_i(\vec{\xi})$ , we have for arbitrary  $B \in \mathcal{B}(R^+)$

$$\begin{aligned} P(T_{j+1}^{i+1} \in B, \xi_{j+1}^{i+1} = \vec{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi_0^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1}) \\ = \int_{T_j^{i+1}}^{\infty} I_B(t_{j+1}) I_{\{t_{j+1} : \pi_{[0,i]}(\vec{\xi}) \in \mathfrak{S}(X^{S_i}(t_{j+1}))\}}(t_{j+1}) \\ \cdot \exp\left\{-\int_{T_j^{i+1}}^{t_{j+1}} |X^{S_i}(t)| dt\right\} dt_{j+1}. \end{aligned}$$

PROOF. See Theorem B.10 in the supplemental article [4].  $\square$

Case 2:  $\xi_j^{i+1} \neq \xi_0^{i+1}$  and  $\pi_i(\xi_j^{i+1}) \neq \emptyset$ . Because the time point at which  $S_{i+1}$  appears is unique, in this case  $T_{j+1}^{i+1}$  must be a jump time of  $X^{S_i}$ . We define

$$(3.17) \quad \mathcal{H} := \inf\{t > T_j^{i+1} : \pi_{[0,i]}(\xi_j^{i+1}) \notin \mathfrak{S}(X^{S_i}(t))\}.$$

THEOREM 6. Suppose that  $\xi_j^{i+1} \neq \xi_0^{i+1}$  and  $\pi_i(\xi_j^{i+1}) \neq \emptyset$ . Then for  $\vec{\xi} \in \mathcal{P}^{i+2}$  satisfying  $\pi_{i+1}(\vec{\xi}) = \pi_{i+1}(\xi_0^{i+1}) \cup \pi_i(\vec{\xi})$ ,  $\pi_i(\xi_j^{i+1}) \subset \pi_i(\vec{\xi})$  and  $\pi_{[0,i]}(\vec{\xi}) \in \mathfrak{S}(X^{S_i}(\mathcal{H}))$ , it holds that

$$P(T_{j+1}^{i+1} = \mathcal{H}, \xi_{j+1}^{i+1} = \vec{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi_0^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1}) = 1,$$

where  $\mathcal{H}$  is defined by (3.17).

PROOF. See Theorem B.11 in the supplemental article [4].  $\square$

Case 3:  $\xi_j^{i+1} \neq \xi_0^{i+1}$  and  $\pi_i(\xi_j^{i+1}) = \emptyset$ . In this case there is a potential recombination which generates again a new lineage carrying  $\xi_0^{i+1}$ . Let  $\mathcal{H}$  be defined by (3.17). If the waiting time is smaller than  $\mathcal{H} - T_j^{i+1}$ , then recombination happens; otherwise no recombination will happen and the lineage which carries  $\xi_j^{i+1}$  will follow the change of  $X^{S_i}$ . In what follows, for an arbitrary  $\vec{\xi} \in \mathcal{P}^{i+2}$ , we define

$$(3.18) \quad h(\vec{\xi}) := \min\{l : \pi_p(\vec{\xi}) = \emptyset, \text{ for all } l < p \leq i\},$$

if  $\pi_i(\vec{\xi}) = \emptyset$ , otherwise we set  $h(\vec{\xi}) := i$ .

THEOREM 7. Suppose that  $\xi_j^{i+1} \neq \xi_0^{i+1}$  and  $\pi_i(\xi_j^{i+1}) = \emptyset$ .

(i) For  $\vec{\xi} = \xi_0^{i+1}$  and  $B \in \mathcal{B}(R^+)$ , we have

$$\begin{aligned} P(T_{j+1}^{i+1} \in B, \xi_{j+1}^{i+1} = \xi_0^{i+1} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi_0^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1}) \\ = \int_{T_j^{i+1}}^{\mathcal{H}} I_B(t_{j+1}) \left( \int_{S_{h(\xi_j^{i+1})+1}}^{S_{i+1}} 2^{-1} \rho p(v) dv \right) \\ \cdot \exp \left\{ -(t_{j+1} - T_j^{i+1}) \int_{S_{h(\xi_j^{i+1})+1}}^{S_{i+1}} 2^{-1} \rho p(v) dv \right\} dt_{j+1}, \end{aligned}$$

where  $h(\xi_j^{i+1})$  is specified by (3.18).

(ii) For  $\vec{\xi} \in \mathcal{P}^{i+2}$  satisfying  $\pi_{i+1}(\vec{\xi}) = \pi_{i+1}(\xi_0^{i+1}) \cup \pi_i(\vec{\xi})$ ,  $\pi_i(\xi_j^{i+1}) \subset \pi_i(\vec{\xi})$  and  $\pi_{[0,i]}(\vec{\xi}) \in \mathfrak{S}(X^{S_i}(\mathcal{H}))$ , we have

$$\begin{aligned} P(T_{j+1}^{i+1} = \mathcal{H}, \xi_{j+1}^{i+1} = \vec{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi_0^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1}) \\ = \exp \left\{ -(\mathcal{H} - T_j^{i+1}) \int_{S_{h(\xi_j^{i+1})+1}}^{S_{i+1}} 2^{-1} \rho p(v) dv \right\}. \end{aligned}$$

(iii) For  $\vec{\xi} \in \mathcal{P}^{i+2}$  satisfying neither (i) nor (ii), we have

$$P(\xi_{j+1}^{i+1} = \vec{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi_0^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1}) = 0.$$

PROOF. See Theorem B.12 in the supplemental article [4].  $\square$

3.2. *Spatial algorithm.* Based on the random sequence  $\{(S_i, Z^i), i \geq 0\}$  discussed above, in this subsection we describe our model of spatially moving algorithm and study its statistical property.

3.2.1. *SC algorithm.* In this subsection, we describe briefly our spatially moving algorithm; for details, see [16]. Our new algorithm is called *SC*, which will recursively construct part graph  $X^{S_i}$  with each branch assigned some label  $k \leq i$ . All the branches with label  $i$  form the local tree  $\mathcal{T}_{S_i}$ .

*Step 1.* Construct a standard Kingman's coalescent tree (cf. [12])  $\mathcal{T}_0$  at the position  $S_0 = 0$  (the left end point of the sequence) and assign each branch of the tree with the label 0. Let  $X^0 = \mathcal{T}_0$ .

*Step 2.* Assume that we have already constructed  $X^{S_i}$  along with local tree  $\mathcal{T}_{S_i}$ . Take the next recombination point  $S_{i+1}$  along the sequence according to the distribution

$$P(S_{i+1} > s | X^{S_i}) = \exp \left\{ -\rho L_{S_i}(X^{S_i}) \int_{S_i}^{s \vee S_i} 2^{-1} p(r) dr \right\}.$$

If  $S_{i+1} \geq 1$ , stop; otherwise, go to step 3.

*Step 3.* Uniformly choose a recombination location on  $\mathcal{T}_{S_i}$ . For  $j = 0$ , let  $T_j^{i+1}$  denote the latitude (i.e., the height from the bottom to the location) of the chosen location.

*Step 4.* At the recombination location, a new branch with label  $i + 1$  is created by forking off the recombination node and moving backward in time (i.e., along the direction of increasing latitude). With equal exponential rate 1, the new branch will have a tendency to coalesce to each branch in  $X^{S_i}$  which has higher latitude than  $T_j^{i+1}$ . Thus, if there are  $l$  branches in  $X^{S_i}$  at the current latitude, then the waiting time before coalescence is exponentially distributed with parameter  $l$ . Note at different latitude there may be different number  $l$  of branches. Let the branch to which the new branch coalesces be called EDGE, and let  $T_{j+1}^{i+1}$  be the latitude of the coalescent point and regard  $j + 1$  as  $j$  in the next step.

*Step 5.* If the EDGE is labeled with  $i$ , go to step 6; if the EDGE is labeled with some  $k$  less than  $i$ , then a potential recombination event should be considered. The waiting time  $t$  of the possible recombination event on the EDGE is exponentially distributed with parameter  $\int_{S_{k+1}}^{S_{i+1}} 2^{-1} \rho p(u) du$ .

- *Case 5.1.* If  $T_j^{i+1} + t$  is less than the latitude of the upper node of the EDGE which is denoted by  $\mathcal{H}$ , then it is the next recombination location. Let  $T_{j+1}^{i+1} = T_j^{i+1} + t$ , the part of the branch above  $T_{j+1}^{i+1}$  is no longer called EDGE. Regard  $j + 1$  as  $j$  and go to step 4.
- *Case 5.2.* If  $T_j^{i+1} + t \geq \mathcal{H}$ , choose the upper edge of the current EDGE with the larger label to be the next EDGE. Let  $T_{j+1}^{i+1} = \mathcal{H}$ , regard  $j + 1$  as  $j$  and go to step 5.

*Step 6.* Let  $X^{S_{i+1}}$  be the collection of all the branches in  $X^{S_i}$  and all the new branches labeled  $i + 1$ . Starting from each node  $1 \leq m \leq N$  at the bottom of the graph, specify a path moving along the edges in  $X^{S_{i+1}}$  increasing latitude, until the top of the graph. Whenever a recombination node is encountered, choose the edge with the larger label. The collection of all the paths then form the local tree  $\mathcal{T}_{S_{i+1}}$ . Update all the branches in  $\mathcal{T}_{S_{i+1}}$  with label  $i + 1$ .

**3.2.2. Some explanation of SC.** Assume that we have already constructed  $X^{S_i}$ . Then the local tree  $\mathcal{T}_{S_i}$  and the breakpoints  $S_1, \dots, S_i$  are all known. Thus, steps 2 and 3 are feasible. Moreover, once we have constructed  $X^{S_i}$ , then the ancestral material of each edge in  $X^{S_i}$ , expressed as an  $(i + 1)$ -dimensional  $\mathcal{P}$ -valued vector [cf. (4.3)], is also implicitly known. In step 4, if we denote by  $\vec{z} = (z_0, z_1, \dots, z_i) \in \mathcal{P}^{i+1}$  the ancestral material of the edge where the recombination location lies, then it is implicitly assumed that the ancestral material carried on the new branch with label  $i + 1$  is the  $(i + 2)$ -dimensional  $\mathcal{P}$ -valued vector  $(\emptyset, \dots, \emptyset, z_i)$ . If for  $j = 0$  we write  $\xi^{i+1}$

for  $z_i$ , and denote  $\xi_0^{i+1} := (\emptyset, \dots, \emptyset, \xi^{i+1})$ , then in steps 4 and 5 the algorithm specifies a path describing how the ancestral material  $\xi_0^{i+1}$  coalesces to  $X^{S_i}$  by coalescence and leaves  $X^{S_i}$  by recombination. When the EDGE in step 4 is labeled  $i$ , then it is implicitly assumed that the path carrying the ancestral material  $\xi_0^{i+1}$  extends continuously along the edges with the larger label in  $X^{S_i}$ , starting from the EDGE until the top of the graph. In step 6, the algorithm formulates  $X^{S_{i+1}}$  with the branches in  $X^{S_i}$  and the new branches created in step 4. For an edge in  $X^{S_i}$  carrying an ancestral material  $(z_0, z_1, \dots, z_i) \in \mathcal{P}^{i+1}$ , when the edge is viewed as an edge in  $X^{S_{i+1}}$ , it is implicitly assumed that its ancestral material is updated to  $(z_0, z_1, \dots, z_i, z_{i+1}) \in \mathcal{P}^{i+2}$  by the following rule: (i) if the edge is on the path of  $\xi_0^{i+1}$  specified above, then  $z_{i+1} = z_i \cup \xi^{i+1}$ ; (ii) if the edge is not on the path of  $\xi_0^{i+1}$ , then  $z_{i+1} = z_i$  on the part of the edge below the latitude  $T_0^{i+1}$ , and  $z_{i+1} = z_i \setminus \xi^{i+1}$  on the part of the edge above the latitude  $T_0^{i+1}$ .

**3.2.3. Distribution of the ARG generated by SC.** In this subsection, we shall show that the probability distribution of the ARG generated by the SC algorithm coincides with that generated by the back-in-time algorithm as specified in Theorem 1. To this end, we denote by  $|Bp|$  the maximum  $i$  such that  $S_i < 1$ . For each  $0 \leq i < |Bp|$ , we denote by  $Z^{i+1}(t)$  the ancestral material [represented as an  $(i+2)$ -dimensional  $\mathcal{P}$ -valued vector] at the latitude  $t \geq T_0^{i+1}$  on the path of edges carrying  $\xi_0^{i+1}$ , and set  $Z^{i+1}(t) = \vec{\emptyset}$  for  $t < T_0^{i+1}$ , with  $\vec{\emptyset}$  representing the null vector in  $\mathcal{P}^{i+2}$ . For  $i \geq |Bp|$ , we set  $S_{i+1} = 1$ ,  $T_0^{i+1} = \infty$ , and  $Z^{i+1}(t) \equiv \vec{\emptyset}$ . Further, we write  $Z^0(t) = \mathcal{T}_0(t)$  for  $t \geq 0$ .

**PROPOSITION 16.** *With the above convention, the finite dimensional distribution of the random sequence  $\{(S_i, Z^i), i \geq 0\}$  generated by the SC algorithm is the same as that developed in Section 3.1.*

Proposition 16 is proved in Section 4.5.

By virtue of the above proposition, we are in a position to prove the following most important theorem of this paper.

**THEOREM 8.** *Let  $(G, \mathcal{B}(G), P)$  be the probability space specified in Theorem 1, and denote by  $\tilde{P}$  the probability distribution on  $G$  generated by SC algorithm. Then we have  $\tilde{P} = P$ .*

Theorem 8 is proved in Section 4.6.

#### 4. Proofs and technical lemmas.

**4.1. Proof of Proposition 14.** The proof of Proposition 14 needs the following lemma.

LEMMA 1. *For each  $i \geq 1$ , we have*

$$(4.1) \quad \mathcal{F}^{S_i} = \sigma(X^0, S_1, \dots, S_i; X^{S_1}, \dots, X^{S_i}) = \sigma(X^{S_i}).$$

PROOF. By the classical theory of jump processes (cf., e.g., [9], Definition 11.48 and Corollary 5.57), we have

$$(4.2) \quad \mathcal{F}^s = \bigcup_{i=0}^{\infty} (\mathcal{G}_i \cap \{S'_i \leq s < S'_{i+1}\})$$

and

$$\mathcal{F}^{S'_i} = \mathcal{G}_i,$$

where  $\mathcal{G}_i = \sigma(X^0, S'_1, \dots, S'_i; X^{S'_1}, \dots, X^{S'_i})$ . Since  $X^s = X^1$  for  $s \geq 1$ , one can check that  $\mathcal{F}^1 = \mathcal{F}^\infty$ ,  $S_i = S'_i \wedge 1$ ,  $\sigma(S_i) = \sigma(S'_i)$  and  $X^{S_i} = X^{S'_i}$  for  $i \geq 1$ . Hence, we have  $\mathcal{G}_i = \sigma(X^0, S_1, \dots, S_i; X^{S_1}, \dots, X^{S_i})$ . Therefore, we have

$$\mathcal{F}^{S_i} = \mathcal{F}^{S'_i} \cap \mathcal{F}^1 = \mathcal{F}^{S'_i} = \sigma(X^0, S_1, \dots, S_i; X^{S_1}, \dots, X^{S_i}).$$

Next, for an arbitrary  $g \in G$ , suppose that  $g(t)$  is expressed as  $g(t) = \{f_1, f_2, \dots, f_k\}$ , then by Proposition 10(v) we can show that

$$(4.3) \quad f_j^{S_i} = \sum_{l=0}^{i-1} \pi_l(\vec{z}_j) I_{[S_l, S_{l+1})} + \pi_i(\vec{z}_j) I_{[S_i, 1)}.$$

Consequently, for  $l \leq i$ , we have  $X^{S_i} = \pi_{[0, S_i]}^G(X^{S_i})$  and  $S_l(g) = S_l(X^{S_i}(g))$ , and the second equality of (4.1) follows.  $\square$

PROOF OF PROPOSITION 14. By (4.3), we have  $Z^l(g) = Z^l(X^{S_i}(g))$  for all  $l \leq i$ , hence

$$\sigma(S_1, \dots, S_i; Z^0, Z^1, \dots, Z^i) \subset \sigma(X^0, S_1, \dots, S_i; X^{S_1}, \dots, X^{S_i}) = \sigma(X^{S_i}).$$

To show the inverse inclusion, we put

$$(4.4) \quad \Omega_i := [0, 1]^i \times \mathcal{S}_{[0, \infty)}(\mathcal{R}) \times \prod_{l=1}^i \mathcal{S}_{[0, \infty)}(\mathcal{P}^{l+1}),$$

where  $\mathcal{R}$  is the collection of all the partitions of  $\{1, 2, \dots, N\}$ , and  $\mathcal{S}_{[0, \infty)}(\mathcal{P}^{l+1})$  [resp.,  $\mathcal{S}_{[0, \infty)}(\mathcal{R})$ ] equipped with the Skorohod topology are the spaces of all the  $\mathcal{P}^{l+1}$ -valued (resp.,  $\mathcal{R}$ -valued) right continuous piecewise constant func-



tions on  $[0, \infty)$  with at most finitely many discontinuity points. Define

$$(4.5) \quad \Phi_i := (S_1, \dots, S_i; Z^0, Z^1, \dots, Z^i).$$

From Propositions 9 and 11, we see that  $\Phi_i$  is a continuous map from  $G$  to the Polish space  $\Omega_i$ . Denote by  $\mathcal{H}_i = \Phi_i(G)$ . By (4.3), we have  $\mathcal{H}_i = \Phi_i(X^{S_i}(G))$ . By (4.3) and Proposition 12 one can check that  $\Phi_i$  restricted to  $X^{S_i}(G)$  is an injective map. Below we write  $G_i := X^{S_i}(G)$ . Note that  $G_i = \{g \in G : g = X^{S_i}(g)\}$  is a Borel subset of the Polish space  $G$ . Hence  $\mathcal{H}_i = \Phi_i(G_i)$  is a Borel subset of  $\Omega_i$  and  $(\Phi_i|_{G_i})^{-1} : \mathcal{H}_i \mapsto G_i$  is Borel measurable (cf. [5], Theorems 8.3.5 and 8.3.7). Define a map  $\Upsilon_i : \Omega_i \mapsto G$  by setting  $\Upsilon_i(\omega) = (\Phi_i|_{G_i})^{-1}(\omega)$  if  $\omega \in \mathcal{H}_i$  and  $\Upsilon_i(\omega) = g_0$  if  $\omega \notin \mathcal{H}_i$ , where  $g_0$  is a fixed element in  $G$ . Since  $(\Phi_i|_{G_i})^{-1}$  is Borel measurable and  $\mathcal{H}_i$  is a Borel subset of  $\Omega_i$ , hence  $\Upsilon_i$  is also Borel measurable. Noticing that  $X^{S_i}(g) = \Upsilon_i(\Phi_i(g))$ , we conclude that  $\sigma(X^{S_i}) \subset \sigma(S_1, \dots, S_i; Z^0, Z^1, \dots, Z^i)$ , completing the proof.  $\square$

4.2. *Proof of Theorem 2.* The proof of Theorem 2 requires the following two lemmas.

LEMMA 2. *For  $0 \leq u < s < 1$ , it holds that*

$$P(\{g : \pi_{[0,s]}^G(g) = \pi_{[0,u]}^G(g)\} | \mathcal{F}^u) = \exp \left\{ -\rho L_u(X^u) \int_u^s 2^{-1} p(r) dr \right\}.$$

PROOF. For  $s \geq 0$ , we set  $\gamma^s := \gamma^s(g) = \inf\{n : \tau_{n+1}^s(g) = \infty\}$ . Note that  $X^s(\cdot)(g) := \pi_{[0,s]}^G(g)$  is uniquely determined by  $\{X^s(0), \tau_1^s, X^s(\tau_1^s), \tau_2^s, X^s(\tau_2^s), \dots\}$ . Therefore for  $0 \leq u < s$ ,  $\pi_{[0,s]}^G(g) = \pi_{[0,u]}^G(g)$  if and only if  $\tau_n^s = \tau_n^u$  and  $X^s(\tau_n^s) = X^u(\tau_n^u)$  for all  $1 \leq n \leq \gamma^u$ , and  $\gamma^s = \gamma^u$ . Write  $G^u = X^u(G)$ . Since  $G^u = \{g \in G : g = \pi_{[0,u]}^G(g)\}$ , hence  $G^u \in \mathcal{B}(G)$ . For  $k \geq 1$ , we set  $A_k = \{g \in G^u : \gamma^u(g^u) = k\}$  and define

$$F_k(g) := (\tau_1^u(g), X^u(\tau_1^u)(g), \dots, \tau_k^u(g), X^u(\tau_k^u)(g))$$

for  $g \in A_k$ . Then  $F_k$  is a measurable map from  $A_k$  to  $B_k := F_k(A_k) \subset (R^+ \times E^u)^k$ . Since  $A_k$  is a Borel subset of the Polish space  $G$  and  $F_k$  is injective,  $B_k$  is a Borel subset of  $(R^+ \times E^u)^k$  (cf., e.g., [5], Theorem 8.3.7). By the one to one correspondence between  $A_k$  and  $B_k$ , one can check that if  $g \in G$  satisfies  $(\tau_1^s(g), X^s(\tau_1^s)(g), \dots, \tau_k^s(g), X^s(\tau_k^s)(g)) \in B_k$ , then  $\pi_{[0,s]}^G(g) = \pi_{[0,u]}^G(g)$ .

For  $A \in \mathcal{B}(G^u)$ ,  $A \subset A_k$ , denote by  $B = F_k(A) \subset B_k$ . Applying Proposition 15, we have

$$\begin{aligned} P(\{g : X^u \in A, \pi_{[0,s]}^G(g) = \pi_{[0,u]}^G(g)\}) \\ = P(\{g : (X^u(0), \tau_1^u, X^u(\tau_1^u), \dots, \tau_k^u, X^u(\tau_k^u)) \in B, \pi_{[0,s]}^G(g) = \pi_{[0,u]}^G(g)\}) \end{aligned}$$

$$\begin{aligned}
&= P(\{g: (X^s(0), \tau_1^s, X^s(\tau_1^s), \dots, \tau_k^s, X^s(\tau_k^s)) \in B\}) \\
&= \int_{R^+ \times E} \cdots \int_{R^+ \times E} \cdots \int_{R^+ \times E} I_B(y_0, t_1, y_1, \dots, t_k, y_k) \\
&\quad \cdot \exp \left\{ - \sum_{n=0}^{k-1} q(y_n, [y_n^s]^c)(t_{n+1} - t_n) \right\} \\
&\quad dt_{k+1} q(y_k, dy_{k+1}) \cdots dt_{n+1} q(y_n, dy_{n+1}) \cdots dt_1 q(y_0, dy_1).
\end{aligned}$$

For  $\omega = (t_1, y_1, \dots, t_k, y_k) \in B_k$ , if we set  $g_\omega := y_0 I_{[0, t_1)}(t) + \sum_{j=1}^k y_j I_{[t_j, t_{j+1})}(t)$ , with the convention that  $t_{k+1} = \infty$ , then  $g_\omega \in G^u$  and it is easy to check that  $L_u(g_\omega) = \sum_{n=0}^{k-1} |\pi_u(y_n)|(t_{n+1} - t_n)$ . Since  $y_n \in E^u$ , by (2.12) we can derive that for  $u < s$ ,  $q(y_n, [y_n^s]^c) = q(y_n, [y_n^u]^c) + |\pi_u(y_n)| \int_u^s 2^{-1} \rho p(r) dr$ . Therefore, from the above we get

$$\begin{aligned}
&P(\{g: X^u \in A, \pi_{[0, s]}^G(g) = \pi_{[0, u]}^G(g)\}) \\
&= \int_{R^+ \times E} \cdots \int_{R^+ \times E} \cdots \int_{R^+ \times E} I_B(y_0, t_1, y_1, \dots, t_k, y_k) \\
&\quad \cdot \exp \left\{ - \sum_{n=0}^{k-1} q(y_n, [y_n^u]^c)(t_{n+1} - t_n) \right\} \\
&\quad \cdot \exp \left\{ - \sum_{n=0}^{k-1} |\pi_u(y_n)|(t_{n+1} - t_n) \int_u^s 2^{-1} \rho p(r) dr \right\} \\
&\quad dt_{k+1} q(y_k, dy_{k+1}) \cdots dt_{n+1} q(y_n, dy_{n+1}) \cdots dt_1 q(y_0, dy_1) \\
&= \int_G I_{\{X^u \in A\}} \exp \left\{ - \rho L_u(X^u) \int_u^s 2^{-1} p(r) dr \right\} P(dg).
\end{aligned}$$

The proof is completed by noticing that  $G = \sum_k A_k$  and  $\mathcal{F}^u = \sigma(X^u)$ .  $\square$

LEMMA 3. For an arbitrary  $(\mathcal{F}^s)$ -stopping time  $\tau$ , we write  $T_\tau = \inf\{s > \tau : X^s \neq X^\tau\}$ , then the distribution of  $T_\tau$  conditioning on  $\mathcal{F}^\tau$  is: for  $s < 1$ ,

$$P(T_\tau > s | \mathcal{F}^\tau) = \exp \left\{ - \rho L_\tau(X^\tau) \int_\tau^{s \vee \tau} 2^{-1} p(r) dr \right\}.$$

PROOF. For  $n \geq 1$ , we define

$$\tau^{(n)} = \sum_{j=1}^{\infty} \frac{j}{2^n} I_{\{(j-1)/2^n \leq \tau < j/2^n\}} + \infty I_{\{\tau = \infty\}}.$$

Then  $\{\tau^{(n)}\}$  are countably valued stopping times and  $\tau^{(n)} \downarrow \tau$ . By the convergence theorem of conditional expectations (cf., e.g., [9], Theorem 2.21),

for  $s < 1$  employing Lemma 2 we obtain

$$\begin{aligned}
P(T_\tau > s | \mathcal{F}^\tau) I_{\{\tau < s\}} &= P(T_\tau > s, \tau < s | \mathcal{F}^\tau) \\
&= \lim_{n \rightarrow \infty} P(T_\tau > s, \tau^{(n)} < s | \mathcal{F}^{\tau^{(n)}}) \\
&= \lim_{n \rightarrow \infty} \sum_{j=1}^{\infty} P(T_\tau > s, j/2^n < s | \mathcal{F}^{j/2^n}) I_{\{\tau^{(n)} = j/2^n\}} \\
&= \lim_{n \rightarrow \infty} \sum_{j/2^n < s} \exp\left(-\rho L_{j/2^n} \int_{j/2^n}^s 2^{-1} p(r) dr\right) I_{\{\tau^{(n)} = j/2^n\}} \\
&= \lim_{n \rightarrow \infty} \exp\left(-\rho L_{\tau^{(n)}} \int_{\tau^{(n)}}^s 2^{-1} p(r) dr\right) I_{\{\tau^{(n)} < s\}} \\
&= \exp\left(-\rho L_\tau \int_\tau^s 2^{-1} p(r) dr\right) I_{\{\tau < s\}}.
\end{aligned}$$

On the other hand, we have

$$\begin{aligned}
P(T_\tau > s | \mathcal{F}^\tau) I_{\{\tau \geq s\}} &= P(T_\tau > s, \tau \geq s | \mathcal{F}^\tau) = P(\tau \geq s | \mathcal{F}^\tau) \\
&= I_{\{\tau \geq s\}} = \exp\left\{-\rho L_\tau \int_\tau^{s \vee \tau} 2^{-1} p(r) dr\right\} I_{\{\tau \geq s\}}. \quad \square
\end{aligned}$$

PROOF OF THEOREM 2. If  $\tau = S_i$ , then we have  $S_{i+1} = T_\tau \wedge 1$ . Therefore, the theorem is a direct consequence of the above lemma.  $\square$

4.3. *Proof of Theorem 3.* Comparing (3.1) and (3.16), it is apparent that  $Z^0(t) = \mathcal{T}_0(t)$ . In Proposition 15, let  $s = u = 0$  and  $k = 0$ , then for  $B \in \mathcal{B}((R^+ \times E^0)^n)$  we have

$$\begin{aligned}
&P\{(\tau_1^0, X^0(\tau_1^0), \dots, \tau_n^0, X^0(\tau_n^0)) \in B\} \\
&= \int_0^\infty dt_1 \cdots \int_0^\infty dt_n \int_E q(y_0, dy_1) \cdots \int_E q(y_{n-1}, dy_n) \\
&\quad \cdot I_{\{t_1 < \dots < t_n\}}(t_1, \dots, t_n) \prod_{j=0}^{n-1} I_{E^0}(y_{j+1}) \\
&\quad \cdot \exp\left\{-\sum_{j=0}^{n-1} q(y_j, [y_j^0]^c)(t_{j+1} - t_j)\right\}.
\end{aligned}$$

Note that  $q(y, [y^0]^c) = |\pi_0^E(y)|(|\pi_0^E(y)| - 1)/2$  for  $y \in E^0$ . Identifying  $y$  with  $\pi_0^E(y)$  for  $y \in E^0$ , we see that  $\{\mathcal{T}_0(t), t \geq 0\}$  is a standard Kingman's coalescent tree.

4.4. *Proof of Theorem 4.* We first make some preparing discussions. For  $0 \leq j \leq k, a \in [0, 1)$  and  $\xi \in \mathcal{P}$ , we put  $A_{k,a,j,\xi} = \{\gamma^a = k, S_i \leq a, \xi \in \mathcal{T}_a(\tau_j^a)\}$ . For notational convenience, below we use also  $A_{k,a,j,\xi}$  to denote the indicator function of  $A_{k,a,j,\xi}$ . For  $j \geq 0, a \in [0, 1), s \in [0, 1), \varepsilon > 0$  and  $\xi \in \mathcal{P}$ , we define

$$(4.6) \quad \begin{aligned} K_{a,s,\varepsilon,j,\xi} &= \{s - \varepsilon \leq S_{i+1} < s, \tau_{j+1}^s \leq t, \tau_j^a < \tau_{j+1}^s < \tau_{j+1}^a, \\ &\exists r \in (s - \varepsilon, s) \text{ and } f \in X^s(\tau_{j+1}^s), \\ &\text{s.t. } f(r) = \xi, f(u) = \emptyset \text{ for all } u < r\}. \end{aligned}$$

LEMMA 4. *Let  $s \in [0, 1)$  and  $\varepsilon > 0$  be such that  $a < s - \varepsilon$ . Then for any  $t > 0$ , we have*

$$\begin{aligned} P(K_{a,s,\varepsilon,j,\xi} | X^a) A_{k,a,j,\xi} \\ = C(a, j, s, \varepsilon) P(\{s - \varepsilon \leq S_{i+1} < s\} | X^a) A_{k,a,j,\xi}, \end{aligned}$$

where

$$(4.7) \quad \begin{aligned} C(a, j, s, \varepsilon) &:= \left(1 - \exp\left\{-\rho L_a \int_{s-\varepsilon}^s 2^{-1} p(r) dr\right\}\right)^{-1} \cdot \int_{s-\varepsilon}^s 2^{-1} \rho p(r) dr \\ &\cdot \int_{\tau_j^a \wedge t}^{\tau_{j+1}^a \wedge t} \exp\left\{-\left[|\mathcal{T}_a(\tau_j^a)|(t' - \tau_j^a) + \sum_{l=0}^{j-1} |\mathcal{T}_a(\tau_l^a)|(\tau_{l+1}^a - \tau_l^a)\right]\right. \\ &\quad \left.\cdot \int_{s-\varepsilon}^s 2^{-1} \rho p(r) dr\right\} dt'. \end{aligned}$$

PROOF. We need only to check the lemma in the case that  $A_{k,a,j,\xi} \neq \emptyset$ . Note that  $A_{k,a,j,\xi} \in \mathcal{F}^a = \sigma(X^a)$ . Take an arbitrary set  $H \in \sigma(X^a)$ . Define  $B = F_k(H \cap A_{k,a,j,\xi})$ , where  $F_k$  is specified as in the proof of Lemma 2. Then  $B \subset (R^+ \times E^a)^k$  and

$$H \cap A_{k,a,j,\xi} = \{g : (\tau_1^a(g), X^a(\tau_1^a)(g), \dots, \tau_k^a(g), X^a(\tau_k^a)(g)) \in B\}.$$

Suppose that  $B \neq \emptyset$ . One can check that

$$(4.8) \quad \begin{aligned} K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi} \\ = \{g : (\tau_1^s, X^s(\tau_1^s), \dots, \tau_j^s, X^s(\tau_j^s), \\ \tau_{j+1}^{s-\varepsilon}, X^{s-\varepsilon}(\tau_{j+1}^{s-\varepsilon}), \dots, \tau_k^{s-\varepsilon}, X^{s-\varepsilon}(\tau_k^{s-\varepsilon})) \in B, \\ \tau_{j+1}^s \leq t, \tau_{j+1}^s < \tau_{j+1}^{s-\varepsilon}, \exists r \in (s - \varepsilon, s) \text{ and } f \in X^s(\tau_{j+1}^s), \\ \text{s.t. } f(r) = \xi, f(u) = \emptyset \text{ for all } u < r\}. \end{aligned}$$

Because  $B \subset F_k(\{\gamma^a = k, \xi \in \mathcal{T}_a(\tau_j^a)\})$ , therefore, for  $(t_1, y_1, \dots, t_j, y_j, \dots, t_k, y_k) \in B$ , there exists  $f_l \in y_j$  such that  $f_l(u) = \xi$  for  $u \in [a, 1]$ . We set

$$J_{y_j} = \{y \in E^s : y = R_{lu}(y_j), u \in (s - \varepsilon, s) \text{ and } l \text{ satisfies } f_l \in y_j, f_l(u) = \xi\}$$

and define

$$B' := \{(t_1, y_1, \dots, t_j, y_j, t', y', t_{j+1}, y_{j+1}, \dots, t_k, y_k) \in (R^+ \times E^s)^{k+1} : \\ (t_1, y_1, \dots, t_j, y_j, \dots, t_k, y_k) \in B, t' \in (t_j, t_{j+1}) \cap (0, t], y' \in J_{y_j}\}.$$

With  $\tau_{j+1}^s, X^s(\tau_{j+1}^s)$  in the place of  $t', y'$ , we may write (4.8) as

$$K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi} \\ = \{g : (\tau_1^s, X^s(\tau_1^s), \dots, \tau_j^s, X^s(\tau_j^s), \tau_{j+1}^s, \\ X^s(\tau_{j+1}^s), \tau_{j+1}^{s-\varepsilon}, X^{s-\varepsilon}(\tau_{j+1}^{s-\varepsilon}), \dots, \tau_k^{s-\varepsilon}, X^{s-\varepsilon}(\tau_k^{s-\varepsilon})) \in B'\}.$$

For  $j+1 \leq l \leq k$ , we set  $\vartheta_l := \tau_{j+1}^s + \tau_{l-j}^{s-\varepsilon} \circ \theta_{\tau_{j+1}^s}$ . One can check that  $\vartheta_l = \tau_l^{s-\varepsilon}$  for each  $l$ . Employing the strong Markov property and Proposition 15, we get

$$P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi}) \\ = \int_0^\infty dt_1 \cdots \int_0^\infty dt_k \int_{t_j \wedge t}^{t_{j+1} \wedge t} dt' \int_E q(y_0, dy_1) \cdots \\ \int_E q(y_{j-1}, dy_j) \int_E q(y_j, dy') \\ \int_E q(\pi_{[0,s-\varepsilon]}^E(y'), dy_{j+1}) \cdots \int_E q(y_{k-1}, dy_k) I_B(t_1, y_1, \dots, t_k, y_k) I_{J_{y_j}}(y') \\ \cdot \exp \left\{ - \sum_{l=0}^{j-1} q(y_l, [y_l^s]^c)(t_{l+1} - t_l) - \sum_{l=j+1}^{k-1} q(y_l, [y_l^{s-\varepsilon}]^c)(t_{l+1} - t_l) \right. \\ \left. - q(y_j, [y_j^s]^c)(t' - t_j) - q(y', [(y')^{s-\varepsilon}]^c)(t_{j+1} - t') \right\}.$$

Since  $y_j \in E^a$ , hence for  $y' \in J_{y_j}$  we have  $\pi_{[0,s-\varepsilon]}^E(y') = \pi_{[0,s-\varepsilon]}^E(y_j) = y_j$  and  $\int_E q(y_j, dy') I_{J_{y_j}}(y') = \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du$ . Therefore,

$$P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi}) \\ = \int_0^\infty dt_1 \cdots \int_0^\infty dt_k \int_E q(y_0, dy_1) \cdots \int_E q(y_{k-1}, dy_k) \\ I_B(t_1, y_1, \dots, t_k, y_k) \int_{t_j \wedge t}^{t_{j+1} \wedge t} dt' \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du$$

$$\cdot \exp \left\{ - \sum_{l=0}^{j-1} q(y_l, [y_l^s]^c)(t_{l+1} - t_l) - \sum_{l=j+1}^{k-1} q(y_l, [y_l^{s-\varepsilon}]^c)(t_{l+1} - t_l) \right. \\ \left. - q(y_j, [y_j^s]^c)(t' - t_j) - q(y_j, [y_j^{s-\varepsilon}]^c)(t_{j+1} - t') \right\}.$$

For  $(t_1, y_1, \dots, t_k, y_k) \in B$ , we have  $y_l \in E^a$  for all  $1 \leq l \leq k$ , therefore,  $q(y_l, [y_l^s]^c) = q(y_l, [y_l^{s-\varepsilon}]^c) + |\pi_a(y_l)| \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du$ . Thus,

$$P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi}) \\ = \int_0^\infty dt_1 \cdots \int_0^\infty dt_k \int_E q(y_0, dy_1) \cdots \int_E q(y_{k-1}, dy_k) \\ I_B(t_1, y_1, \dots, t_k, y_k) \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \int_{t_j \wedge t}^{t_{j+1} \wedge t} dt' \\ \cdot \exp \left\{ - \sum_{l=0}^{j-1} \left[ q(y_l, [y_l^{s-\varepsilon}]^c) + |\pi_a(y_l)| \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \right] (t_{l+1} - t_l) \right. \\ \left. - \sum_{l=j+1}^{k-1} q(y_l, [y_l^{s-\varepsilon}]^c)(t_{l+1} - t_l) - q(y_j, [y_j^{s-\varepsilon}]^c)(t_{j+1} - t') \right. \\ \left. - \left[ q(y_j, [y_j^{s-\varepsilon}]^c) + |\pi_a(y_j)| \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \right] (t' - t_j) \right\}.$$

Note that  $q(y_l, [y_l^{s-\varepsilon}]^c) = q(y_l, [y_l^a]^c) + |\pi_a(y_l)| \int_a^{s-\varepsilon} 2^{-1} \rho p(u) du$ . We define  $\tilde{L}_a := \sum_{l=0}^{k-1} (t_{l+1} - t_l) |\pi_a(y_l)|$ , then

$$P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi}) \\ = \int_0^\infty dt_1 \cdots \int_0^\infty dt_k \int_E q(y_0, dy_1) \cdots \int_E q(y_{k-1}, dy_k) \\ I_B(t_1, y_1, \dots, t_k, y_k) \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \int_{t_j \wedge t}^{t_{j+1} \wedge t} dt' \\ \cdot \exp \left\{ - \sum_{l=0}^{k-1} q(y_l, [y_l^a]^c)(t_{l+1} - t_l) - 2^{-1} \rho \tilde{L}_a \int_a^{s-\varepsilon} p(u) du \right. \\ \left. - \sum_{l=0}^{j-1} |\pi_a(y_l)| (t_{l+1} - t_l) \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \right. \\ \left. - |\pi_a(y_j)| (t' - t_j) \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \right\}.$$

Multiplying with  $(1 - \exp\{-\tilde{L}_a \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du\}) / (1 - \exp\{-\tilde{L}_a \times \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du\})$  at the right-hand side of the above equality, we get

$$\begin{aligned} & P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi}) \\ &= \int_0^\infty dt_1 \cdots \int_0^\infty dt_k \int_E q(y_0, dy_1) \cdots \int_E q(y_{k-1}, dy_k) I_B(t_1, y_1, \dots, t_k, y_k) \\ & \quad \cdot \exp\left\{-\sum_{l=0}^{k-1} q(y_l, [y_l^a]^c)(t_{l+1} - t_l)\right\} \tilde{C}(t_1, y_1, \dots, t_k, y_k) \\ & \quad \cdot \left[\exp\left(-2^{-1} \rho \tilde{L}_a \int_a^{s-\varepsilon} p(u) du\right) - \exp\left(-2^{-1} \rho \tilde{L}_a \int_a^s p(u) du\right)\right], \end{aligned}$$

where

$$\begin{aligned} & \tilde{C}(t_1, y_1, \dots, t_k, y_k) \\ &:= \left(1 - \exp\left\{-\tilde{L}_a \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du\right\}\right)^{-1} \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du \\ & \quad \cdot \int_{t_j \wedge t}^{t_{j+1} \wedge t} \exp\left\{-\left[|\pi_a(y_j)|(t' - t_j) + \sum_{l=0}^{j-1} |\pi_a(y_l)|(t_{l+1} - t_l)\right]\right. \\ & \quad \left. \cdot \int_{s-\varepsilon}^s 2^{-1} \rho p(u) du\right\} dt'. \end{aligned}$$

For  $\omega = (t_1, y_1, \dots, t_k, y_k) \in B$ , if we set  $g_\omega := y_0 I_{[0,t_1)}(t) + \sum_{l=1}^k y_l I_{[t_l, t_{l+1})}(t)$ , with the convention that  $t_{k+1} = \infty$ , then  $g_\omega \in G^a$ . One can check that  $|\mathcal{T}_a(\tau_l^a)|(g_\omega) = |\pi_a(y_l)|$ ,  $L_a(g_\omega) = \sum_{l=0}^{k-1} |\pi_a(y_l)|(t_{l+1} - t_l) = \tilde{L}_a$  and  $C(a, j, s, \varepsilon)(g_\omega) = \tilde{C}(t_1, y_1, \dots, t_k, y_k)$ . Therefore, applying Proposition 15 we obtain

$$\begin{aligned} & P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi}) \\ &= \int_H C(a, j, s, \varepsilon) \left[ \exp\left(-2^{-1} \rho L_a \int_a^{s-\varepsilon} p(u) du\right) \right. \\ & \quad \left. - \exp\left(-2^{-1} \rho L_a \int_a^s p(u) du\right) \right] A_{k,a,j,\xi} P(dg). \end{aligned}$$

Since  $H \in \sigma(X^a)$  is arbitrary, hence what we have proved implies that

$$\begin{aligned} & P(K_{a,s,\varepsilon,j,\xi} \cap H \cap A_{k,a,j,\xi} | X^a) \\ &= C(a, j, s, \varepsilon) \left[ \exp\left(-2^{-1} \rho L_a \int_a^{s-\varepsilon} p(u) du\right) \right. \\ & \quad \left. - \exp\left(-2^{-1} \rho L_a \int_a^s p(u) du\right) \right] A_{k,a,j,\xi} \end{aligned}$$



$$= C(a, j, s, \varepsilon) P(\{s - \varepsilon \leq S_{i+1} < s\} | X^a) A_{k,a,j,\xi},$$

where the last line is due to Lemma 3. The proof is completed by noticing that  $A_{k,a,j,\xi} \in \sigma(X^a)$ .  $\square$

For  $n \geq 1$ , we define  $\sigma_n = 2^{-n}([2^n S_{i+1}] + 1)$ . Then each  $\sigma_n$  is a countably valued  $\{\mathcal{F}^s\}$  stopping time and  $\sigma(S_{i+1}) = \bigvee_n \sigma(\sigma_n)$ . If we replace  $s$  by  $\sigma_n$  and  $\varepsilon$  by  $2^{-n}$  in (4.6), we get another subset  $\tilde{K}_{a,\sigma_n,j,\xi}$  from the expression of  $K_{a,s,\varepsilon,j,\xi}$  as follows:

$$(4.9) \quad \begin{aligned} \tilde{K}_{a,\sigma_n,j,\xi} &= \{\tau_{j+1}^{\sigma_n} \leq t, \tau_j^a < \tau_{j+1}^{\sigma_n} < \tau_{j+1}^a, \exists r \in (\sigma_n - 2^{-n}, \sigma_n) \\ &\text{and } f \in X^{\sigma_n}(\tau_{j+1}^{\sigma_n}), \text{ s.t. } f(r) = \xi, f(u) = \emptyset \text{ for all } u < r\}. \end{aligned}$$

LEMMA 5. *Let the notation be the same as the above lemma. For any  $n \geq 1$  and  $t > 0$ , we have*

$$\begin{aligned} P(\tilde{K}_{a,\sigma_n,j,\xi} | X^a, \sigma_n) A_{k,a,j,\xi} I_{\{a < \sigma_n - 1/2^n\}} \\ = C\left(a, j, \sigma_n, \frac{1}{2^n}\right) A_{k,a,j,\xi} I_{\{a < \sigma_n - 1/2^n\}}. \end{aligned}$$

PROOF. By the definition of  $\sigma_n$ , we have  $\sigma_n = \sum_{m \geq 1} \frac{m}{2^n} I_{\{m/2^n - 1/2^n \leq S_{i+1} < m/2^n\}}$ , hence  $\tilde{K}_{a,\sigma_n,j,\xi} = \bigcup_{m \geq 1} K_{a,m/2^n,1/2^n,j,\xi}$ . Then by Lemma 4 one can check directly that

$$\begin{aligned} P(\tilde{K}_{a,\sigma_n,j,\xi} | X^a, \sigma_n) A_{k,a,j,\xi} I_{\{a < \sigma_n - 1/2^n\}} \\ = \sum_{m \geq 1} P(K_{a,m/2^n,1/2^n,j,\xi} | X^a) \left( P\left(\left\{\frac{m}{2^n} - \frac{1}{2^n} \leq S_{i+1} < \frac{m}{2^n}\right\} \middle| X^a\right) \right)^{-1} \\ \cdot A_{k,a,j,\xi} I_{\{a < m/2^n - 1/2^n\}} I_{\{m/2^n - 1/2^n \leq S_{i+1} < m/2^n\}} \\ = \sum_{m \geq 1} C\left(a, j, \frac{m}{2^n}, \frac{1}{2^n}\right) A_{k,a,j,\xi} I_{\{a < m/2^n - 1/2^n\}} I_{\{\sigma_n = m/2^n\}} \\ = C\left(a, j, \sigma_n, \frac{1}{2^n}\right) A_{k,a,j,\xi} I_{\{a < \sigma_n - 1/2^n\}}. \quad \square \end{aligned}$$

PROOF OF THEOREM 4. For  $m \geq 1$ , we define  $\alpha_m = 2^{-m}([2^m S_i] + 1)$ . If we replace  $a$  by  $\alpha_m$  in  $\tilde{K}_{a,\sigma_n,j,\xi}$ , we get another subset  $\tilde{K}_{\alpha_m,\sigma_n,j,\xi}$ . Similar to the proof of Lemma 5, we can show that

$$\begin{aligned} P(\tilde{K}_{\alpha_m,\sigma_n,j,\xi} | X^{\alpha_m}, \sigma_n) A_{k,\alpha_m,j,\xi} I_{\{\alpha_m < \sigma_n - 1/2^n\}} \\ = C\left(\alpha_m, j, \sigma_n, \frac{1}{2^n}\right) A_{k,\alpha_m,j,\xi} I_{\{\alpha_m < \sigma_n - 1/2^n\}}. \end{aligned}$$

Since  $\lim_{m \rightarrow \infty} \alpha_m = S_i$  and  $\sigma(S_i) = \bigvee_m \sigma(\alpha_m)$ , by the convergence property of conditional expectations (cf., e.g., [9], Theorem 2.21), we get

$$(4.10) \quad \begin{aligned} & P(\tilde{K}_{S_i, \sigma_n, j, \xi} | X^{S_i}, \sigma_n) A_{k, S_i, j, \xi} I_{\{S_i < \sigma_n - 1/2^n\}} \\ &= C\left(S_i, j, \sigma_n, \frac{1}{2^n}\right) A_{k, S_i, j, \xi} I_{\{S_i < \sigma_n - 1/2^n\}}. \end{aligned}$$

Note that by (4.7) we have

$$\lim_{n \rightarrow \infty} C\left(S_i, j, \sigma_n, \frac{1}{2^n}\right) = \frac{1}{L_{S_i}} \int_{\tau_j^{S_i} \wedge t}^{\tau_{j+1}^{S_i} \wedge t} du.$$

By the definition of  $A_{k, S_i, j, \xi}$ , we have

$$A_{k, S_i, j, \xi} = \{\gamma^{S_i} = k, \xi \in \mathcal{T}_{S_i}(\tau_j^{S_i})\}.$$

Noticing that  $\tilde{K}_{S_i, \sigma_n, j, \xi} \rightarrow \{T_0^{i+1} \leq t, \xi^{i+1} = \xi, T_0^{i+1} \in (\tau_j^{S_i}, \tau_{j+1}^{S_i})\}$  a.s. as  $n \rightarrow \infty$ , letting  $n \rightarrow \infty$  in the both sides of (4.10) and employing again the convergence property of conditional expectations, we get

$$\begin{aligned} & P\{T_0^{i+1} \leq t, \xi^{i+1} = \xi, T_0^{i+1} \in (\tau_j^{S_i}, \tau_{j+1}^{S_i}) | X^{S_i}, S_{i+1}\} I_{\{\gamma^{S_i} = k, \xi \in \mathcal{T}_{S_i}(\tau_j^{S_i})\}} \\ &= \frac{1}{L_{S_i}} \int_{\tau_j^{S_i} \wedge t}^{\tau_{j+1}^{S_i} \wedge t} du I_{\{\gamma^{S_i} = k, \xi \in \mathcal{T}_{S_i}(\tau_j^{S_i})\}}. \end{aligned}$$

Summing up the above equation for  $k$  and  $j$ , and noticing that  $\xi \in \mathcal{T}_{S_i}(\tau_j^{S_i})$  if and only if  $\xi \in \mathcal{T}_{S_i}(u)$  for all  $\tau_j^{S_i} \leq u < \tau_{j+1}^{S_i}$ , we complete the proof of the theorem.  $\square$

**4.5. Proof of Proposition 16.** By Theorem 3, we see that the distribution of  $Z^0$  generated by step 1 coincides the distribution of  $Z^0$  defined by (3.1). It is apparent that the conditional distribution of  $S_{i+1}$  generated by step 2 coincides with the one specified by Theorem 2, and the conditional distribution of  $T_0^{i+1}$  and  $\xi^{i+1}$  generated by step 3 is the same as those described by Theorem 4. To analyze the random elements generated in steps 4 and 5, we define recursively for  $n \geq 1$ ,

$$(4.11) \quad T_n^i = \inf\{t > T_{n-1}^i : Z^i(t) \neq Z^i(T_{n-1}^i)\} \quad \text{and} \quad \xi_n^i = Z^i(T_n^i).$$

In step 4, it is implicitly assumed that the ancestral material carried on the new branch is  $\xi_0^{i+1}$ , which means that  $\xi_j^{i+1} = \xi_0^{i+1}$ . It is not difficult to check that the distribution employed in step 4 coincides with the one developed in Theorem 5. To analyze step 5, we note that step 5 corresponds to the case that  $\xi_j^{i+1} \neq \xi_0^{i+1}$ , and the EDGE is labeled with  $i$  if and only if

$\pi_i(\xi_j^{i+1}) \neq \emptyset$ . When the EDGE is labeled with  $i$ , the algorithm goes to step 6, the path carrying the ancestral material  $\xi_0^{i+1}$  is assumed to move along the edges of  $X^{S_i}$ . In this case,  $T_{j+1}^{i+1}$  must be the jump time of  $X^{S_i}$  at which the lineage carrying the ancestral material  $\pi_{[0,i]}(\xi_j^{i+1})$  meets its first change after  $T_j^{i+1}$ . Thus, the conditional distribution of  $(T_n^{i+1}, \xi_n^{i+1})$  coincides with the one described in Theorem 6. In step 5, when the EDGE is labeled with some  $k$  less than  $i$ , then a potential recombination event is considered in the algorithm. We point out that  $k$  is equal to  $h(\vec{\xi}_j)$  used in Theorem 7, and the upper node of the EDGE, denoted by  $\mathcal{H}$  in the algorithm, is the time point  $\mathcal{H}$  used in Theorem 7. Then one can check that the distribution used in step 5 coincides with the conditional distribution developed in Theorem 7. To sum up the above discussion, we find that all the distributions of the random elements generated by the algorithm coincide with those developed in Section 3.1. Therefore, the finite dimensional distribution of the random sequence  $\{(S_i, Z^i), i \geq 0\}$  generated by the  $SC$  algorithm is the same as that developed in Section 3.1.

4.6. *Proof of Theorem 8.* Below we use  $\{(\tilde{S}_i, \tilde{Z}^i), i \geq 0\}$  to denote the random elements  $\{(S_i, Z^i), i \geq 0\}$  generated by the  $SC$  algorithm, and reserve  $\{(S_i, Z^i), i \geq 0\}$  for those originally defined on  $(G, \mathcal{B}(G), P)$  as discussed in Section 3.1. It is implicitly assumed that  $\{(\tilde{S}_i, \tilde{Z}^i), i \geq 0\}$  are taken from some probability space other than the space  $G$ . We denote by

$$(4.12) \quad \tilde{\Phi}_i := (\tilde{S}_1, \dots, \tilde{S}_i; \tilde{Z}^0, \tilde{Z}^1, \dots, \tilde{Z}^i),$$

and denote by  $\tilde{P}_i$  the probability distribution of  $\tilde{\Phi}_i$  on its sample space  $\Omega_i$  specified by (4.4). Here,

$$\Omega_i := [0, 1]^i \times \mathcal{S}_{[0, \infty)}(\mathcal{R}) \times \prod_{l=1}^i \mathcal{S}_{[0, \infty)}(\mathcal{P}^{l+1})$$

is also the sample space of  $\Phi_i := (S_1, \dots, S_i; Z^0, Z^1, \dots, Z^i)$  specified by (4.5). Denote by  $P_i$  the probability distribution of  $\Phi_i$ . By Proposition 16, we have  $\tilde{P}_i = P_i$ . Bellow we use the notation employed in the proof of Proposition 14. Then  $\tilde{P}_i = P_i$  implies in particular that  $\tilde{P}_i(\mathcal{H}_i) = 1$ . Each  $\omega \in \mathcal{H}_i$  constitutes a part graph  $g \in X^{S_i}(G) := G_i$ , which is described by the map  $\Upsilon_i := (\Phi_i|_{G_i})^{-1}$ . Since  $\Upsilon_i: \mathcal{H}_i \mapsto G_i$  is a one to one Borel map, hence  $\tilde{P}_i$  induces a probability measure  $\tilde{P}_i^* = \tilde{P}_i \circ (\Upsilon_i)^{-1}$  on  $G_i$ . Similarly,  $P_i$  induces a probability measure  $P_i^*$  on  $G_i$  and we have  $\tilde{P}_i^* = P_i^*$ . By Lemma 1, we have  $\sigma(X^{S_i}) = \mathcal{F}^{S_i}$ . For notational convenience below, we write  $\mathcal{F}_i$  for  $\mathcal{F}^{S_i}$ . Through the mapping  $X^{S_i}: G_i \mapsto G$ , the probability measure  $P_i^*$  determines a probability measure  $P_{|\mathcal{F}_i}^*$  on  $(G, \mathcal{F}_i)$  by setting  $P_{|\mathcal{F}_i}^*((X^{S_i})^{-1}(B)) = P_i^*(B)$  for all  $B \in \mathcal{B}(G_i)$ .

Noticing that  $X^{S_i}(g) = \Upsilon_i(\Phi_i(g))$ , one can check that  $P|_{\mathcal{F}_i}^* = P|_{\mathcal{F}_i}$  where  $P|_{\mathcal{F}_i}$  is the restriction of  $P$  on  $\mathcal{F}_i$ . Similarly,  $\tilde{P}_i^*$  determines a probability measure  $\tilde{P}|_{\mathcal{F}_i}^*$  on  $(G, \mathcal{F}_i)$ . On the other hand, let  $\tilde{P}$  be the probability distribution on  $(G, \mathcal{B}(G))$  generated by the algorithm  $SC$ , then we must have  $\tilde{P} \circ (X^{S_i})^{-1} = \tilde{P}_i^*$  on  $G_i$ . Then it is clear that  $\tilde{P}|_{\mathcal{F}_i}^* = \tilde{P}|_{\mathcal{F}_i}$ . Therefore, we get  $\tilde{P}|_{\mathcal{F}_i} = \tilde{P}|_{\mathcal{F}_i}^* = P|_{\mathcal{F}_i}^* = P|_{\mathcal{F}_i}$ . The proof of the theorem is completed by noticing that  $\mathcal{B}(G) = \bigvee_{i \geq 1} \mathcal{F}_i$ .

**Aknowledgments.** We are indebted to Shuhua Xu, Ying Zhou, Linfeng Li and Yuting Liu for allowing us to use some material from our joint work [16]. We are grateful to De-Xin Zhang and Wei-Wei Zhai for offering their stimulating idea and for their encouragement. We thank Renming Song for his very helpful comments and suggestions. We thank the Editor, Associate Editor and the anonymous referees for their valuable comments and suggestions which improved the presentation of this paper.

## SUPPLEMENTARY MATERIAL

**Supplement to “Markov jump processes in modeling coalescent with recombination”** (DOI: [10.1214/14-AOS1227SUPP](https://doi.org/10.1214/14-AOS1227SUPP); .pdf). The supplementary file is divided into two Appendixes. Appendix A contains the proofs of Propositions 1–9 and Propositions 11–13. Appendix B is devoted to the calculation of the conditional distribution  $P(T_{j+1}^{i+1} \in B, \xi_{j+1}^{i+1} = \tilde{\xi} | X^{S_i}, S_{i+1}, T_0^{i+1}, \xi^{i+1}, \dots, T_j^{i+1}, \xi_j^{i+1})$ . In particular, the proofs of Theorems 5, 6 and 7 are presented, respectively, in the proofs of Theorems B.10, B.11 and B.12 in Appendix B.

## REFERENCES

- [1] CHEN, G. K., MARJORAM, P. and WALL, J. D. (2009). Fast and flexible simulation of DNA sequence data. *Genome. Res.* **19** 136–142.
- [2] CHEN, M.-F. (2004). *From Markov Chains to Non-Equilibrium Particle Systems*, 2nd ed. World Scientific, River Edge, NJ. [MR2091955](#)
- [3] CHEN, X. and MA, Z. M. (2014). A transformation of Markov jump processes and applications in genetic study. *Discrete Contin. Dyn. Syst. Ser. A.* **34** To appear.
- [4] CHEN, X., MA, Z. and WANG, Y. (2014). Supplement to “Markov jump processes in modeling coalescent with recombination.” DOI:[10.1214/14-AOS1227SUPP](https://doi.org/10.1214/14-AOS1227SUPP).
- [5] COHN, D. L. (1980). *Measure Theory*. Birkhäuser, Boston, MA. [MR0578344](#)
- [6] ETHIER, S. N. and KURTZ, T. G. (1986). *Markov Processes: Characterization and Convergence*. Wiley, New York. [MR0838085](#)
- [7] GRIFFITHS, R. C. and MARJORAM, P. (1996). Ancestral inference from samples of DNA sequences with recombination. *J. Comput. Biol.* **3** 479–502.
- [8] GRIFFITHS, R. C. and MARJORAM, P. (1997). An ancestral recombination graph. In *Progress in Population Genetics and Human Evolution* (P. DONNELLY and S. TAVARÉ, eds.). *The IMA Volumes in Mathematics and Its Applications* **87** 100–117. Springer, Berlin.

- [9] HE, S. W., WANG, J. G. and YAN, J. A. (1992). *Semimartingale Theory and Stochastic Calculus*. Science Press, Beijing. [MR1219534](#)
- [10] HUDSON, R. R. (1983). Properties of a neutral allele model with intragenic recombination. *Theor. Popul. Biol.* **23** 183–201.
- [11] HUDSON, R. R. (2002). Generating samples under a Wright–Fisher neutral model of genetic variation. *Bioinformatics* **18** 337–338.
- [12] KINGMAN, J. F. C. (1982). The coalescent. *Stochastic Process. Appl.* **13** 235–248. [MR0671034](#)
- [13] KINGMAN, J. F. C. (1982). On the genealogy of large populations. *J. Appl. Probab.* **19A** 27–43. [MR0633178](#)
- [14] MARJORAM, P. and WALL, J. D. (2006). Fast “coalescent” simulation. *BMC Genet.* **7** 16.
- [15] MCVEAN, G. A. T. and CARDIN, N. J. (2005). Approximating the coalescent with recombination. *Philos. Trans. R. Soc. Lond., B, Biol. Sci.* **360** 1387–1393.
- [16] WANG, Y., ZHOU, Y., LI, L. F., CHEN, X., LIU, Y. T., MA, Z. M. and XU, S. H. (2013). A new method for modeling coalescent processes with recombination. Preprint.
- [17] WATTERSON, G. A. (1975). On the number of segregating sites in genetical models without recombination. *Theor. Popul. Biol.* **7** 256–276. [MR0366430](#)
- [18] WIUF, C. and HEIN, J. (1999). Recombination as a point process along sequences. *Theor. Popul. Biol.* **55** 248–259.

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